A Stable, Convergent, Conservative and Linear Finite Difference Scheme for the Cahn-Hilliard Equation

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We propose a stable, convergent, conservative and linear finite difference scheme to solve numerically the Cahn-Hilliard equation. The proposed scheme realizes both linearity and stability. We show uniqueness, existence and convergence of the solution to the scheme. Numerical examples demonstrate the effectiveness of the proposed scheme.

Key words: finite difference method, linear scheme, decrease of energy, conservation of mass, Cahn-Hilliard equation

1. Introduction

The Cahn-Hilliard equation [2]

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{\delta G}{\delta u}\right), \qquad x \in (0, L) \subset \mathbf{R},\ 0 < t \tag{1.1}$$

$$\frac{\delta G}{\delta u} = pu + ru^3 + q\,\frac{\partial^2 u}{\partial x^2}, \tag{1.2}$$

with initial condition $u(x, 0) = u_0(x)$, where p, q and r are constants with $p < 0$, $q < 0$ and $0 < r$, is a model equation to describe a phase separation phenomenon called the spinodal decomposition. The decomposition phenomenon occurs when binary solutions such as alloys, polymer mixtures are cooled down [19]. Here $u(x, t)$ is a distribution function of the concentration of one component of the binary mixture. Boundary conditions for the equation are

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} = 0, \tag{1.3}$$

$$\left.\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right|_{x=0} = \left.\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right|_{x=L} = 0, \tag{1.4}$$

i.e.,

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} = 0, \tag{1.5}$$

$$\left.\frac{\partial^3 u}{\partial x^3}\right|_{x=0} = \left.\frac{\partial^3 u}{\partial x^3}\right|_{x=L} = 0. \tag{1.6}$$

The functional G means a local free energy called the Ginzburg-Landau free energy. The notation $\frac{\delta G}{\delta u}$ defined by (1.2) is consistent with the variational derivative of

$$G(u(x,t)) = \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q\left(\frac{\partial u}{\partial x}\right)^2 \tag{1.7}$$

with respect to $u(x,t)$. In fact, a relation between G of (1.7) and $\frac{\delta G}{\delta u}$ of (1.2),

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{\int_0^L G(u+\epsilon v)dx - \int_0^L G(u)dx\right\} = \int_0^L v\frac{\delta G}{\delta u}\,dx, \tag{1.8}$$

is derived through integration by parts under the boundary condition (1.3).

It is known that the solution $u(x,t)$ of the Cahn-Hilliard equation possesses the properties that the total mass $\int_0^L u(x,t)dx$ is conserved and that the total free energy $\int_0^L G(u(x,t))dx$ decreases with time. Steady state solutions of the Cahn-Hilliard equation were studied by Carr, Gurtin and Slemrod [3] and Novick-Cohen and Segel [17]. Elliott and Zheng [9] proved that if the initial data $u(x,0)$ belongs to

$$H_E^2(\Omega) \equiv \left\{f \in H^2(\Omega);\ \frac{\partial f}{\partial \nu} = 0 \ \text{ on } \ \partial\Omega\right\}, \tag{1.9}$$

then the Cahn-Hilliard equation has a unique solution $u(x,t) \in H^{4,1}(\Omega \times (0,T))$ where Ω is a bounded domain in $\mathbf{R}^n$ $(n \le 3)$ and $\partial/\partial\nu$ is the outward normal derivative to $\partial\Omega$. In spite of these studies, there remains a lot to be investigated, e.g. how the solution $u(x,t)$ evolves and attains to a final state.

Since we cannot hope for analytical solutions, we must resort to numerical methods to solve the Cahn-Hilliard equation. Even numerical solutions are not easy to obtain because this equation is a nearly ill-posed problem when $p < 0$. To overcome this difficulty, some numerical methods have been considered in several papers. Langer, Bar-on and Milners made a pioneering study [15] based on a simple ansatz for the two-point distribution function. Some finite element schemes were studied with mathematical rigor by Elliott and Sonqmu [9], Elliott and French [5], Elliott, French and Milner [7], Elliott and French [6] and Elliott and Larsson [8]. Du and Nicolaides [4] proposed an interesting finite element scheme and a finite difference scheme with the property that the total energy decreases with time under the Dirichlet boundary conditions. Furihata, Onda and Mori [14] proposed a practical nonlinear stability analysis method for finite difference schemes and applied it to the Cahn-Hilliard equation. Sun [18] proposed an interesting linearized finite difference scheme which is uniquely solvable and L_2-convergent, not necessarily stable. In [11] Furihata proposed another difference scheme for the Cahn-Hilliard equation based on the discrete variational derivative technique [10]. The scheme in [11] is conservative, stable and L_2-convergent, but implicit with nonlinearity.

In this paper we design a new linear finite difference scheme for the Cahn-Hilliard equation based on a combination of the discrete variational derivative technique in [12], [10] and the linearization technique in [16]. The proposed linear scheme is stable and L_2-convergent, and inherits the conservation of mass and the decrease of the total energy from the Cahn-Hilliard equation. From the mass conservation and the energy decrease properties, we show that the scheme is stable in the sense that the numerical solution is bounded with respect to max-norm. It is proven that the proposed scheme has a unique solution under a certain mild condition for Δt. It is also proven that the numerical solution by the proposed scheme converges to the true solution of the Cahn-Hilliard equation with the convergence rate of $O\left((\Delta x)^2 + (\Delta t)^2\right)$ if $u(x,\cdot) \in C^3[0,T]$ for any fixed x and $u(\cdot,t) \in C^6[0,L]$ for any fixed t, where $u(x,t)$ is the true solution. Finally some numerical examples are shown to demonstrate the effectiveness of the proposed difference scheme. It is observed that the proposed difference scheme is stable even when Δt is 1000 times as large as the stability upper limit of Δt in the conventional schemes reported in [14].

2. Discrete Symbols and Discrete Calculus

In this section we introduce a consistent set of discrete operators.

We suppose that the space mesh size Δx and the time mesh size Δt are uniform. First, we define a general rule to compose the m-th operator $\mathrm{o}^{\langle m\rangle}$ from a given pair of commutative operators o^+ and o^- as follows:

$$\mathrm{o}^{\langle 0\rangle} \stackrel{\text{def}}{=} 1, \tag{2.1}$$

$$\mathrm{o}^{\langle 1\rangle} \stackrel{\text{def}}{=} \frac{1}{2}(\mathrm{o}^+ + \mathrm{o}^-), \tag{2.2}$$

$$\mathrm{o}^{\langle 2\rangle} \stackrel{\text{def}}{=} \mathrm{o}^+\mathrm{o}^-, \tag{2.3}$$

$$\mathrm{o}^{\langle 2m+1\rangle} \stackrel{\text{def}}{=} \mathrm{o}^{\langle 1\rangle}\mathrm{o}^{\langle 2m\rangle}, \qquad m \geq 1, \tag{2.4}$$

$$\mathrm{o}^{\langle 2m+2\rangle} \stackrel{\text{def}}{=} \mathrm{o}^{\langle 2\rangle}\mathrm{o}^{\langle 2m\rangle}, \qquad m \geq 1. \tag{2.5}$$

Next, we define some basic operators, the shift operators s^+, s^-, the average operators μ^+, μ^- and the difference operators δ^+, δ^- with respect to subscript j.

$$s_j^+ f(j) \stackrel{\text{def}}{=} f(j+1), \qquad s_j^- f(j) \stackrel{\text{def}}{=} f(j-1), \tag{2.6}$$

$$\mu_j^+ \stackrel{\text{def}}{=} \frac{s_j^+ + 1}{2}, \qquad \mu_j^- \stackrel{\text{def}}{=} \frac{s_j^- + 1}{2}, \tag{2.7}$$

$$\delta_j^+ \stackrel{\text{def}}{=} \frac{s_j^+ - 1}{\Delta j}, \qquad \delta_j^- \stackrel{\text{def}}{=} \frac{s_j^- - 1}{-\Delta j}, \tag{2.8}$$

where Δj is a generic notation for the mesh size. We use n for time subscript and k for space subscript and define

$$\Delta n \stackrel{\text{def}}{=} \Delta t, \tag{2.9}$$

$$\Delta k \stackrel{\text{def}}{=} \Delta x. \tag{2.10}$$

The generic rules (2.1)–(2.5) applied to $\sigma^\pm = s^\pm$, $\mu^\pm$ and $\delta^\pm$, yield $s^{\langle m \rangle}$, $\mu^{\langle m \rangle}$ and $\delta^{\langle m \rangle}$, respectively.

As a discretization of the integral we adopt the summation $\sum''$ defined by

$$\sum_{k=0}^{N}{}'' f_k \stackrel{\text{def}}{=} \frac{1}{2} f_0 + \sum_{k=1}^{N-1} f_k + \frac{1}{2} f_N. \tag{2.11}$$

Two relationships between difference operators and summations are mentioned. The first is the inverse relationship between difference operators and summation operators for any $h > 0$, $h \in \mathbf{N}$. This reads

$$\sum_{k=0}^{N}{}'' \left(\delta_k^{\langle h \rangle} f_k\right) \Delta x = \left[\mu_k^{\langle h \bmod 2 \rangle} \delta_k^{\langle h-1 \rangle} f_k\right]_{k=0}^{N}, \tag{2.12}$$

where

$$[f_k]_{k=0}^{N} \stackrel{\text{def}}{=} f_N - f_0, \tag{2.13}$$

$$h \bmod 2 = \begin{cases} 0 & : h \text{ is even} \\ 1 & : h \text{ is odd}. \end{cases} \tag{2.14}$$

The second is "summation by parts" that corresponds to integration by parts:

$$\sum_{k=0}^{N}{}'' f_k \left(\delta_k^+ g_k\right) \Delta x + \sum_{k=0}^{N}{}'' \left(\delta_k^- f_k\right) g_k \Delta x = \left[\frac{f_k \left(s_k^+ g_k\right) + \left(s_k^- f_k\right) g_k}{2}\right]_{k=0}^{N}. \tag{2.15}$$

3. The Proposed Scheme

We define $U_k^{(n)}$ ($k = -2, -1, 0, \ldots, N, N+1, N+2$; $n = 0, 1, 2, \ldots$) to be the approximation to $u(x,t)$ at location $x = k\Delta x$ and time $t = n\Delta t$, where $N \stackrel{\text{def}}{=} L/\Delta x$. The concrete form of the proposed linear scheme for (1.1)–(1.2) is

$$\frac{U_k^{(1)} - u_0(k\Delta x)}{\Delta t} = \frac{\partial^2}{\partial x^2} \left(\frac{\delta G(u_0(x))}{\delta u} \right) \Bigg|_{x = k\Delta x}, \tag{3.1}$$

$$\delta_n^{\langle 1 \rangle} U_k^{(n)} = \delta_k^{\langle 2 \rangle} V_k^{(n)}, \quad n = 1, 2, \ldots, \tag{3.2}$$

$$V_k^{(n)} = pU_k^{(n)} + r\big(s_n^{\langle 1\rangle}U_k^{(n)}\big)\big(U_k^{(n)}\big)^2 + q\,\delta_k^{\langle 2\rangle}\big(s_n^{\langle 1\rangle}U_k^{(n)}\big), \tag{3.3}$$

where $U_k^{(0)} = u_0(k\Delta x)$, $k = 0, 1, \ldots, N$. The discrete boundary conditions are

$$U_{-1}^{(n)} = U_1^{(n)}, \qquad U_{N+1}^{(n)} = U_{N-1}^{(n)}, \tag{3.4}$$

$$U_{-2}^{(n)} = U_2^{(n)}, \qquad U_{N+2}^{(n)} = U_{N-2}^{(n)}, \tag{3.5}$$

for $n = 0, 1, 2, \ldots$. These conditions correspond to (1.5) and (1.6). Note that these conditions satisfy

$$\delta_k^{\langle 1\rangle}U_k^{(n)}\Big|_{k=0} = \delta_k^{\langle 1\rangle}U_k^{(n)}\Big|_{k=N} = 0, \tag{3.6}$$

$$\delta_k^{\langle 1\rangle}V_k^{(n)}\Big|_{k=0} = \delta_k^{\langle 1\rangle}V_k^{(n)}\Big|_{k=N} = 0, \tag{3.7}$$

which correspond to (1.3) and (1.4).

From the concrete form of the proposed scheme (3.1), (3.2) and (3.3), it is easy to see that the scheme is linear in the new time step. The proposed scheme is implicit in that we must solve simultaneous linear equations per iteration to obtain numerical solutions. However, the computation time to solve them is proportional to N since the coefficient matrix, which is described in (6.3), is a band matrix.

4. Properties Inherited by the Proposed Scheme

We first note two well-known properties [9] of the solution of the Cahn-Hilliard equation, which are mentioned in the introduction. Namely,

$$\int_0^L u(x,t)dx = \int_0^L u(x,0)dx, \tag{4.1}$$

$$\frac{d}{dt}\int_0^L G(u(x,t))dx \le 0. \tag{4.2}$$

We call (4.1) the conservation of mass and (4.2) the decrease of total energy. The conservation of mass (4.1) can be shown easily as follows:

$$\frac{d}{dt}\int_0^L u(x,t)dx = \int_0^L \frac{\partial u(x,t)}{\partial t}dx = \int_0^L \frac{\partial^2}{\partial x^2}\frac{\delta G}{\delta u}dx = \left[\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right]_{x=0}^L = 0, \tag{4.3}$$

in which the boundary condition (1.4) is used. The decrease of total energy (4.2) can be shown similarly under the same condition:

$$\frac{d}{dt}\int_0^L G(u(x,t))dx = \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}dx = -\int_0^L \left\{\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right\}^2 dx \le 0. \tag{4.4}$$

The main purpose of this section is to show that the proposed scheme (3.1)–(3.3) has properties corresponding respectively to (4.1) and (4.2), i.e.,

$$\sum_{k=0}^{N}{}'' U_k^{(n)} \Delta x = \begin{cases} \sum_{k=0}^{N}{}'' U_k^{(0)} \Delta x, & : n \text{ is even} \\ \sum_{k=0}^{N}{}'' U_k^{(1)} \Delta x, & : n \text{ is odd} \end{cases} \tag{4.5}$$

$$\sum_{k=0}^{N}{}'' G_d\big(U^{(n+1)}, U^{(n)}\big)_k \Delta x - \sum_{k=0}^{N}{}'' G_d\big(U^{(n)}, U^{(n-1)}\big)_k \Delta x \le 0, \tag{4.6}$$

where

$$\begin{aligned} G_d(f,g)_k \stackrel{\text{def}}{=} & \frac{1}{2} p f_k g_k + \frac{1}{4} r (f_k)^2 (g_k)^2 \\ & - \frac{1}{2} q \left(\frac{\big(\delta_k^+ f_k\big)^2 + \big(\delta_k^- f_k\big)^2 + \big(\delta_k^+ g_k\big)^2 + \big(\delta_k^- g_k\big)^2}{4} \right) \end{aligned} \tag{4.7}$$

is the discrete local free energy defined for a pair of vectors $f = \{f_k\}$, $g = \{g_k\}$. We call (4.5) the conservation of discrete mass and (4.6) the decrease of discrete total energy. The conservation of discrete mass (4.5) can be shown as

$$\begin{aligned} \frac{1}{2\Delta t} \left\{ \sum_{k=0}^{N}{}'' U_k^{(n+1)} \Delta x - \sum_{k=0}^{N}{}'' U_k^{(n-1)} \Delta x \right\} &= \sum_{k=0}^{N}{}'' \left\{ \delta_n^{\langle 1 \rangle} U_k^{(n)} \right\} \Delta x \\ &= \sum_{k=0}^{N}{}'' \left\{ \delta_k^{\langle 2 \rangle} V_k^{(n)} \right\} \Delta x \\ &= \left[\delta_k^{\langle 1 \rangle} V_k^{(n)} \right]_{k=0}^{N} \\ &= 0 \end{aligned} \tag{4.8}$$

because of (2.12) and the boundary condition (3.7). The decrease of discrete total energy (4.6) can be shown as

$$\begin{aligned} & \frac{1}{\Delta t} \left\{ \sum_{k=0}^{N}{}'' G_d\big(U_k^{(n+1)}, U_k^{(n)}\big)_k \Delta x - \sum_{k=0}^{N}{}'' G_d\big(U_k^{(n)}, U_k^{(n-1)}\big)_k \Delta x \right\} \\ & = \sum_{k=0}^{N}{}'' \left\{ V_k^{(n)} \delta_n^{\langle 1 \rangle} U_k^{(n)} \right\} \Delta x \\ & = \sum_{k=0}^{N}{}'' \left\{ V_k^{(n)} \delta_k^{\langle 2 \rangle} V_k^{(n)} \right\} \Delta x \end{aligned}$$

$$= \left[s_k^{\langle 1 \rangle} V_k^{(n)} \cdot \delta_k^{\langle 1 \rangle} V_k^{(n)} \right]_{k=0}^{N} - \frac{1}{2} \sum_{k=0}^{N}{}'' \left[\left\{ \delta_k^+ V_k^{(n)} \right\}^2 + \left\{ \delta_k^- V_k^{(n)} \right\}^2 \right] \Delta x$$

$$= -\frac{1}{2} \sum_{k=0}^{N}{}'' \left[\left\{ \delta_k^+ V_k^{(n)} \right\}^2 + \left\{ \delta_k^- V_k^{(n)} \right\}^2 \right] \Delta x$$

$$\le 0, \tag{4.9}$$

because of a relation between G_d and $V_k^{(n)}$ given by

$$\begin{aligned} &\sum_{k=0}^{N}{}'' G_d\big(U^{(n+1)}, U^{(n)}\big)_k \Delta x - \sum_{k=0}^{N}{}'' G_d\big(U^{(n)}, U^{(n-1)}\big)_k \Delta x \\ &\quad = \sum_{k=0}^{N}{}'' \left\{ V_k^{(n)} \left(\frac{U_k^{(n+1)} - U_k^{(n-1)}}{2} \right) \right\} \Delta x + \left[\partial V_k^{(n)} \right]_{k=0}^{N} \\ &\quad = \sum_{k=0}^{N}{}'' \left\{ V_k^{(n)} \left(\frac{U_k^{(n+1)} - U_k^{(n-1)}}{2} \right) \right\} \Delta x, \end{aligned} \tag{4.10}$$

where

$$\begin{aligned} \partial V_k^{(n)} \stackrel{\text{def}}{=} \frac{-q}{8} \Big\{ & \delta_k^+ \big(s_n^{\langle 1 \rangle} U_k^{(n)} \big) \cdot s_k^+ \big(U_k^{(n+1)} - U_k^{(n-1)} \big) \\ & + \delta_k^- \big(s_n^{\langle 1 \rangle} U_k^{(n)} \big) \cdot s_k^- \big(U_k^{(n+1)} - U_k^{(n-1)} \big) \\ & + 2 \delta_k^{\langle 1 \rangle} \big(s_n^{\langle 1 \rangle} U_k^{(n)} \big) \cdot \big(U_k^{(n+1)} - U_k^{(n-1)} \big) \Big\}. \end{aligned} \tag{4.11}$$

The boundary terms in (4.9) and (4.10) vanish because of (3.4) and (3.7). It is noted that the summation by parts (2.15) is used repeatedly in (4.10).

5. Stability of the Proposed Scheme

The purpose of this section is to show that, if the proposed scheme has a solution, it is bounded in the maximum norm. The proof consists of two lemmas. The first lemma shows that the discrete semi-norm of the solution of the proposed difference scheme is bounded. The second shows that if the discrete semi-norm of a discrete function is bounded, so is the maximum norm.

LEMMA 5.1. *The solutions* $U_k^{(n)}$, $n = 0, 1, \ldots$, *of the scheme* (3.1)–(3.3) *under the boundary conditions* (3.4), (3.5) *satisfy*:

$$\sum_{k=0}^{N-1} \big(\delta_k^+ U_k^{(n)}\big)^2 \Delta x \le \left(\frac{4}{-q} \right) \left\{ \sum_{k=0}^{N}{}'' G_d\big(U^{(1)}, U^{(0)}\big)_k \Delta x + \frac{p^2 L}{4r} \right\}. \tag{5.1}$$

Proof. Applying $(r/4)x^2 + (p/2)x \geq -p^2/4r$ to the discrete local free energy in (4.7) we obtain:

$$\begin{aligned}
&\sum_{k=0}^{N}{}'' G_d\big(U^{(n+1)}, U^{(n)}\big)_k \Delta x \\
&\geq \sum_{k=0}^{N}{}'' \left\{ -\frac{p^2}{4r} - \frac{q}{8}\left((\delta_k^+ U_k^{(n+1)})^2 + (\delta_k^- U_k^{(n+1)})^2 + (\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2 \right) \right\} \Delta x \\
&\geq \sum_{k=0}^{N}{}'' \left\{ -\frac{p^2}{4r} - \frac{q}{8}\left((\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2 \right) \right\} \Delta x \\
&= -\frac{p^2}{4r} L - \frac{q}{4} \sum_{k=0}^{N-1} (\delta_k^+ U_k^{(n)})^2 \Delta x, \qquad (5.2)
\end{aligned}$$

since

$$\sum_{k=0}^{N}{}'' \left\{ \left((\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2 \right) \right\} \Delta x = 2 \sum_{k=0}^{N-1} (\delta_k^+ U_k^{(n)})^2 \Delta x \qquad (5.3)$$

under the discrete boundary conditions (3.4), (3.5). The inequality (5.1) follows from the above inequality and the decrease of total energy (4.6). □

LEMMA 5.2. *For any $f = \{f_k\}_{k=0}^{N}$ and $0 \leq {}^\forall m \leq N$, the following inequality is satisfied*:

$$\frac{1}{L}\left(f_m - \frac{M}{L} \right)^2 \leq \sum_{k=0}^{N-1} \left(\delta_k^+ f_k \right)^2 \Delta x, \qquad (5.4)$$

where

$$M \stackrel{\text{def}}{=} \sum_{k=0}^{N}{}'' f_k \Delta x. \qquad (5.5)$$

Proof. For any m such that $0 \leq m \leq N$ we have

$$f_m L - M = \sum_{k=0}^{N}{}'' \left(f_m - f_k \right) \Delta x = \sum_{k=0}^{N}{}'' \gamma_{k,m}(f) \Delta x, \qquad (5.6)$$

where

$$\gamma_{k,m}(f) \stackrel{\text{def}}{=} \begin{cases} \displaystyle\sum_{l=k}^{m-1} \left(\delta_l^+ f_l \right) \Delta x & : \ k \leq m, \\ \displaystyle -\sum_{l=m}^{k-1} \left(\delta_l^+ f_l \right) \Delta x & : \ m < k. \end{cases} \qquad (5.7)$$

This implies

$$\left| f_m - M/L \right| \leq \sum_{k=0}^{N-1} \left| \delta_k^+ f_k \right| \Delta x, \qquad (5.8)$$

since

$$\left|f_m L - M\right| \le \sum_{k=0}^{N}{}'' \left|\gamma_{k,m}(f)\right| \Delta x, \tag{5.9}$$

$$\left|\gamma_{k,m}(f)\right| \le \sum_{k=0}^{N-1} \left|\delta_k^+ f_k\right| \Delta x. \tag{5.10}$$

Finally, applying the Schwartz inequality to (5.8) we obtain the inequality (5.4). □

REMARK. The inequality (5.8) corresponds to the Poincaré-Wirtinger inequality [1, p. 146].

Applying Lemma 5.2 to (5.1) we obtain the following theorem. The inequality (5.11) in the theorem implies that the proposed difference scheme (3.1)–(3.3) is stable for any time step n since the constants U_C^+, U_C^- and ΔU are determined by the initial state.

THEOREM 5.3. *The solutions* $U_k^{(n)}$, $n = 1, 2, \ldots$, *of the scheme* (3.1)–(3.3) *under the boundary conditions* (3.4), (3.5) *satisfy*

$$U_C^- - \Delta U \le U_k^{(n)} \le U_C^+ + \Delta U, \tag{5.11}$$

where

$$U_C^+ \stackrel{\text{def}}{=} \frac{1}{L} \max\left(\sum_{k=0}^{N}{}'' U_k^{(0)} \Delta x, \sum_{k=0}^{N}{}'' U_k^{(1)} \Delta x \right), \tag{5.12}$$

$$U_C^- \stackrel{\text{def}}{=} \frac{1}{L} \min\left(\sum_{k=0}^{N}{}'' U_k^{(0)} \Delta x, \sum_{k=0}^{N}{}'' U_k^{(1)} \Delta x \right), \tag{5.13}$$

$$\Delta U \stackrel{\text{def}}{=} \left[\left(\frac{4L}{-q} \right) \left\{ \sum_{k=0}^{N}{}'' G_d\left(U^{(1)}, U^{(0)}\right)_k \Delta x + \frac{p^2 L}{4r} \right\} \right]^{1/2}. \tag{5.14}$$

Theorem 5.3 is essentially independent of both Δx and Δt except for the dependence of the constants U_C^+, U_C^- and ΔU on Δx and Δt. This means that the proposed scheme (3.1)–(3.3) is unconditionally stable.

REMARK. The influence of rounding-error is not considered in evaluating the stability of the numerical solution.

6. Unique Existence of the Solution to the Proposed Scheme

This section is to prove that the proposed scheme (3.2) has a unique solution under a certain condition on Δt and Δx.

The equation (3.1) has a unique solution without any condition. The equations (3.2), (3.3) can be rewritten as simultaneous linear equations

$$\left\langle 1 - 2\Delta t\left[\frac{r}{2\Delta x^2}\left\{\left(U_{k+1}^{(n)}\right)^2 s_k^+ - 2\left(U_k^{(n)}\right)^2 + \left(U_{k-1}^{(n)}\right)^2 s_k^-\right\} + \frac{q}{2}\delta_k^{\langle 4\rangle}\right]\right\rangle U_k^{(n+1)}$$
$$= 2\Delta t\delta_k^{\langle 2\rangle}\left\{pU_k^{(n)} + \frac{r}{2}\left(U_k^{(n)}\right)^2 U_k^{(n-1)}\right\} + \left(1 + \Delta t q\delta_k^{\langle 4\rangle}\right)U_k^{(n-1)}. \tag{6.1}$$

Under the discrete boundary conditions (3.4), (3.5), the above simultaneous linear equations are written as

$$A\,U^{(n+1)} = w, \tag{6.2}$$

where A is an $(N+1)\times(N+1)$ matrix and $w = \{w_k\}_{k=0}^N$ is a vector with $w_k \stackrel{\text{def}}{=}$ RHS of (6.1). The elements $A_{ij}(0 \le i,\ j \le N)$ of the matrix A are

$$A_{ij} = \begin{cases} 1 + a_i^{(n)} & : i = j,\ i \ne 1,\ i \ne N-1, \\ b_j^{(n)} & : i = j \pm 1,\ i \ne 0,\ i \ne N, \\ c & : i = j \pm 2,\ i \ne 0,\ i \ne N, \\ 1 + a_i^{(n)} + c & : (i,j) = (1,1), (N-1,N-1), \\ 2b_j^{(n)} & : (i,j) = (0,1), (N,N-1), \\ 2c & : (i,j) = (0,2), (N,N-2), \\ 0 & : \text{otherwise}, \end{cases} \tag{6.3}$$

where

$$a_k^{(n)} \stackrel{\text{def}}{=} \Delta t\left\{\frac{2r}{(\Delta x)^2}\left(U_k^{(n)}\right)^2 - \frac{6q}{(\Delta x)^4}\right\}, \quad k = 0,1,\ldots,N, \tag{6.4}$$

$$b_k^{(n)} \stackrel{\text{def}}{=} \Delta t\left\{-\frac{r}{(\Delta x)^2}\left(U_k^{(n)}\right)^2 + \frac{4q}{(\Delta x)^4}\right\}, \quad k = 0,1,\ldots,N, \tag{6.5}$$

$$c \stackrel{\text{def}}{=} \frac{-q\Delta t}{(\Delta x)^4}. \tag{6.6}$$

We obtain the following theorem.

THEOREM 6.1. *When*

$$\Delta t < \frac{-4q}{r^2 \max\left\{\left(U_C^- - \Delta U\right)^4, \left(U_C^+ + \Delta U\right)^4\right\}} \tag{6.7}$$

the proposed scheme (3.1)–(3.3) *has a unique solution.*

Proof. Suppose that $A\boldsymbol{u} = \boldsymbol{0}$ for a non-zero vector $\boldsymbol{u} = \{u_k\}_{k=0}^N$. Note that $A\boldsymbol{u} = \boldsymbol{0}$ is equivalent to the following equality through (6.1):

$$u_k - r\Delta t\,\delta_k^{\langle 2\rangle}\left\{\left(U_k^{(n)}\right)^2 u_k\right\} - q\Delta t\,\delta_k^{\langle 4\rangle} u_k = 0, \quad \text{for } k = 0,1,\ldots N, \tag{6.8}$$

where $u_{-s} \stackrel{\text{def}}{=} u_s$, $u_{N+s} \stackrel{\text{def}}{=} u_{N-s}$ for $s = 1, 2$. Multiplying by u_k, summing from 0 to N, and using summation-by-parts we obtain

$$\sum_{k=0}^{N}{}'' (u_k)^2 \Delta x = r\Delta t \sum_{k=0}^{N}{}'' \left(U_k^{(n)}\right)^2 u_k \delta_k^{\langle 2\rangle} u_k \Delta x + q\Delta t \sum_{k=0}^{N}{}'' \left(\delta_k^{\langle 2\rangle} u_k\right)^2 \Delta x. \tag{6.9}$$

The formula of summation-by-parts used above is

$$\sum_{k=0}^{N}{}'' f_k \delta_k^{\langle 2\rangle} g_k \Delta x = \sum_{k=0}^{N}{}'' g_k \delta_k^{\langle 2\rangle} f_k \Delta x \quad \text{for } \boldsymbol{f},\ \boldsymbol{g} \text{ satisfying (3.4).} \tag{6.10}$$

For the first term of RHS(6.9) we obtain

$$\begin{aligned}
& r\Delta t \sum_{k=0}^{N}{}'' \left(U_k^{(n)}\right)^2 u_k \delta_k^{\langle 2\rangle} u_k \Delta x \\
&= \Delta t \sum_{k=0}^{N}{}'' \left\{\frac{r}{\sqrt{-2q}} \left(U_k^{(n)}\right)^2 u_k\right\} \left\{\sqrt{-2q}\,\delta_k^{\langle 2\rangle} u_k\right\} \Delta x \\
&\le \frac{\Delta t}{2} \sum_{k=0}^{N}{}'' \left[\left\{\frac{r}{\sqrt{-2q}} \left(U_k^{(n)}\right)^2 u_k\right\}^2 + \left\{\sqrt{-2q}\,\delta_k^{\langle 2\rangle} u_k\right\}^2\right] \Delta x \\
&\le \frac{r^2 \Delta t}{-4q} \sum_{k=0}^{N}{}'' \left(U_k^{(n)}\right)^4 (u_k)^2 \Delta x - q\Delta t \sum_{k=0}^{N}{}'' \left(\delta_k^{\langle 2\rangle} u_k\right)^2 \Delta x.
\end{aligned} \tag{6.11}$$

From Theorem 5.3, (6.9) and this inequality (6.11) we obtain

$$\begin{aligned}
\sum_{k=0}^{N}{}'' (u_k)^2 \Delta x &\le \frac{r^2 \Delta t}{-4q} \sum_{k=0}^{N}{}'' \left(U_k^{(n)}\right)^4 (u_k)^2 \Delta x \\
&\le \frac{r^2 \Delta t}{-4q} \max\left\{\left(U_C^- - \Delta U\right)^4, \left(U_C^+ + \Delta U\right)^4\right\} \sum_{k=0}^{N}{}'' (u_k)^2 \Delta x.
\end{aligned} \tag{6.12}$$

Because the vector $\boldsymbol{u}$ is non-zero, this inequality means

$$\frac{-4q}{r^2 \max\left\{\left(U_C^- - \Delta U\right)^4, \left(U_C^+ + \Delta U\right)^4\right\}} \le \Delta t. \tag{6.13}$$

Hence the matrix A is non-singular under the condition (6.7). □

REMARK. For the uniqueness and existence of the numerical solution in Theorem 6.1, the stability theorem (Theorem 5.3) is essential.

7. Error Estimates for the Proposed Scheme

The purpose of this section is to establish an L_2-error estimate of numerical solutions $U_k^{(n)}$ of the proposed scheme. The L_2-error estimate implies that the solution to the scheme (3.1)–(3.3) converges to the solution to the original equation (1.1)–(1.2).

We define the following notations for $n = 0, 1, \dots$ and $k = -2, -1, \dots, N+2$:

$$v(x,t) \stackrel{\mathrm{def}}{=} \frac{\delta G(u(x,t))}{\delta u}, \tag{7.1}$$

$$\tilde{u}_k^{(n)} \stackrel{\mathrm{def}}{=} u_k^{(n)} - U_k^{(n)}, \tag{7.2}$$

$$\tilde{v}_k^{(n)} \stackrel{\mathrm{def}}{=} v_k^{(n)} - V_k^{(n)}, \tag{7.3}$$

$$r_k^{(n)} \stackrel{\mathrm{def}}{=} \delta_n^{\langle 1\rangle} \tilde{u}_k^{(n)} - \delta_k^{\langle 2\rangle} \tilde{v}_k^{(n)}, \tag{7.4}$$

$$h_k^{(n)} \stackrel{\mathrm{def}}{=} \left(u_k^{(n)}\right)^3 - \left(\frac{U_k^{(n+1)} + U_k^{(n-1)}}{2}\right)\left(U_k^{(n)}\right)^2, \tag{7.5}$$

$$f_k^{(n)} \stackrel{\mathrm{def}}{=} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x=k\Delta x,\, t=n\Delta t} - \delta_k^{\langle 2\rangle}\left(\frac{u_k^{(n+1)} + u_k^{(n-1)}}{2}\right), \tag{7.6}$$

where $U_k^{(n)}$ is the solution of the proposed scheme (3.1)–(3.3), $V_k^{(n)}$ is defined in (3.3), $u(x,t)$ is the solution to the Cahn-Hilliard equation, $u_k^{(n)} \stackrel{\mathrm{def}}{=} u(k\Delta x, n\Delta t)$, $v_k^{(n)} \stackrel{\mathrm{def}}{=} v(k\Delta x, n\Delta t)$. We define an extension of u by

$$u(x,t) \stackrel{\mathrm{def}}{=} \begin{cases} u(x-2lL,t) : 2lL \le x \le (2l+1)L, \\ u(2lL-x,t) : (2l-1)L < x < 2lL, \end{cases} \tag{7.7}$$

where $l \in \mathbf{Z}$. We define the extension of v similarly.

Under the discrete boundary conditions (3.4), (3.5) and above definitions, we obtain the following inequality from the summation by parts (2.15):

$$\begin{aligned}
&\frac{1}{2\Delta t}\sum_{k=0}^{N}{}'' \left\{\left(\tilde{u}_k^{(n+1)}\right)^2 - \left(\tilde{u}_k^{(n-1)}\right)^2\right\}\Delta x = 2\sum_{k=0}^{N}{}'' \left(s_n^{\langle 1\rangle}\tilde{u}_k^{(n)} \cdot \delta_n^{\langle 1\rangle}\tilde{u}_k^{(n)}\right)\Delta x \\
&= 2\sum_{k=0}^{N}{}'' \left(s_n^{\langle 1\rangle}\tilde{u}_k^{(n)}\right)\left(\delta_k^{\langle 2\rangle}\tilde{v}_k^{(n)} + r_k^{(n)}\right)\Delta x \\
&= 2\sum_{k=0}^{N}{}'' \left\{\tilde{v}_k^{(n)}\left(\delta_k^{\langle 2\rangle} s_n^{\langle 1\rangle}\tilde{u}_k^{(n)}\right) + s_n^{\langle 1\rangle}\tilde{u}_k^{(n)} \cdot r_k^{(n)}\right\}\Delta x \\
&= 2\sum_{k=0}^{N}{}'' \left\{\tilde{v}_k^{(n)} \cdot \frac{1}{q}\left(\tilde{v}_k^{(n)} - p\tilde{u}_k^{(n)} - rh_k^{(n)} - qf_k^{(n)}\right) + s_n^{\langle 1\rangle}\tilde{u}_k^{(n)} \cdot r_k^{(n)}\right\}\Delta x
\end{aligned}$$

$$= 2\sum_{k=0}^{N}{}'' \left[\frac{1}{q}\left(\tilde{v}_k^{(n)}\right)^2 + \frac{1}{-q}\left(\sqrt{2}\tilde{v}_k^{(n)}\right) \cdot \left\{\frac{1}{\sqrt{2}}\left(p\tilde{u}_k^{(n)} + rh_k^{(n)} + qf_k^{(n)}\right)\right\} + s_n^{\langle 1\rangle}\tilde{u}_k^{(n)} \cdot r_k^{(n)}\right]\Delta x$$

$$\leq 2\sum_{k=0}^{N}{}'' \left[\frac{1}{q}\left(\tilde{v}_k^{(n)}\right)^2 + \frac{1}{-q}\frac{2\left(\tilde{v}_k^{(n)}\right)^2 + \frac{1}{2}\left(p\tilde{u}_k^{(n)} + rh_k^{(n)} + qf_k^{(n)}\right)^2}{2} + s_n^{\langle 1\rangle}\tilde{u}_k^{(n)} \cdot r_k^{(n)}\right]\Delta x$$

$$\leq 2\sum_{k=0}^{N}{}'' \left[\frac{3}{-4q}\left\{\left(p\tilde{u}_k^{(n)}\right)^2 + \left(rh_k^{(n)}\right)^2 + \left(qf_k^{(n)}\right)^2\right\} + \frac{\left(\tilde{u}_k^{(n+1)}\right)^2 + \left(\tilde{u}_k^{(n-1)}\right)^2}{4} + \frac{\left(r_k^{(n)}\right)^2}{2}\right]\Delta x. \tag{7.8}$$

With notation

$$\varepsilon^{(n)} \stackrel{\text{def}}{=} \sum_{k=0}^{N}{}'' \left(\tilde{u}_k^{(n)}\right)^2 \Delta x, \tag{7.9}$$

the above inequality is written as:

$$\frac{\varepsilon^{(n+1)} - \varepsilon^{(n-1)}}{\Delta t} \leq \frac{3p^2}{-q}\varepsilon^{(n)} + \varepsilon^{(n+1)} + \varepsilon^{(n-1)} + \sum_{k=0}^{N}{}'' \left\{\frac{3r^2}{-q}\left(h_k^{(n)}\right)^2 - 3q\left(f_k^{(n)}\right)^2 + 2\left(r_k^{(n)}\right)^2\right\}\Delta x. \tag{7.10}$$

Since the solution of the proposed scheme is bounded as shown in Theorem 5.3, we can evaluate $h_k^{(n)}$ when $u \in C^0([0, L] \times [0, T])$ as follows:

$$\left(h_k^{(n)}\right)^2 \leq 3\Lambda^4\left[\frac{\Delta t^4}{4}\left(\delta_n^{\langle 2\rangle} u_k^{(n)}\right)^2 + \frac{\left(\tilde{u}_k^{(n+1)}\right)^2 + \left(\tilde{u}_k^{(n-1)}\right)^2}{2} + 4\left(\tilde{u}_k^{(n)}\right)^2\right], \tag{7.11}$$

where

$$\Lambda \stackrel{\text{def}}{=} \max\left\{\sup_{\substack{0\leq x\leq L\\ 0\leq t\leq T}} |u(x,t)|,\ \left|U_C^- - \Delta U\right|,\ \left|U_C^+ + \Delta U\right|\right\}, \tag{7.12}$$

and $T \geq (n+1)\Delta t$. Substituting the above estimate into the inequality (7.10) we obtain

$$\left\{1 - \Delta t\left(1 + \frac{9r^2\Lambda^4}{-2q}\right)\right\}\varepsilon^{(n+1)} \leq \left\{1 + \Delta t\left(1 + \frac{9r^2\Lambda^4}{-2q}\right)\right\}\varepsilon^{(n-1)} + \frac{3\Delta t}{-q}\left(p^2 + 12r^2\Lambda^4\right)\varepsilon^{(n)} + \Delta t\sum_{k=0}^{N}{}'' \left\{\frac{9r^2\Lambda^4\Delta t^4}{-4q}\left(\delta_n^{\langle 2\rangle} u_k^{(n)}\right)^2 - 3q\left(f_k^{(n)}\right)^2 + 2\left(r_k^{(n)}\right)^2\right\}\Delta x. \tag{7.13}$$

We now assume that the time mesh size Δt satisfies

$$0 \le \Delta t \le \frac{1}{3}\left(\frac{1}{1+\frac{9r^2\Lambda^4}{-2q}}\right). \tag{7.14}$$

Since

$$0 \le \Delta t \le 1/3a \implies \frac{1+a\Delta t}{1-a\Delta t} \le 1+3a\Delta t, \tag{7.15}$$

it then follows from (7.13) that

$$\begin{aligned}\varepsilon^{(n+1)} &\le \left\{1+3\Delta t\left(1+\frac{9r^2\Lambda^4}{-2q}\right)\right\}\varepsilon^{(n-1)} + \frac{9\Delta t}{-2q}\left(p^2+12r^2\Lambda^4\right)\varepsilon^{(n)} \\ &\quad + \Delta t \sum_{k=0}^{N}{}'' \left\{\frac{27r^2\Lambda^4\Delta t^4}{-8q}\big(\delta_n^{\langle 2\rangle}u_k^{(n)}\big)^2 - \frac{9q}{2}\big(f_k^{(n)}\big)^2 + 3\big(r_k^{(n)}\big)^2\right\}\Delta x. \end{aligned} \tag{7.16}$$

If $u(x,\cdot) \in C^3[0,T]$ for any fixed x and $u(\cdot,t) \in C^6[0,L]$ for any fixed t, the constant

$$C_0 \stackrel{\text{def}}{=} \sup_{x,t}\max\left(\left|\frac{\partial^2 u}{\partial t^2}\right|, \frac{1}{6}\left|\frac{\partial^3 u}{\partial t^3}\right|, \frac{1}{12}\left|\frac{\partial^4 u}{\partial x^4}\right|, \frac{1}{12}\left|\frac{\partial^4 v}{\partial x^4}\right|, \frac{1}{2}\left|\frac{\partial^2}{\partial x^2}\frac{\partial^2}{\partial t^2}u\right|\right) \tag{7.17}$$

satisfies that

$$\left|r_k^{(n)}\right| \le C_0\left((\Delta x)^2 + (\Delta t)^2\right), \tag{7.18}$$

$$\left|f_k^{(n)}\right| \le C_0\left((\Delta x)^2 + (\Delta t)^2\right), \tag{7.19}$$

$$\left|\delta_n^{\langle 2\rangle}u_k^{(n)}\right| \le C_0, \tag{7.20}$$

and we can evaluate the remaining term of the last inequality as follows:

$$\begin{aligned}&\Delta t \sum_{k=0}^{N}{}'' \left\{\frac{27r^2\Lambda^4\Delta t^4}{-8q}\big(\delta_n^{\langle 2\rangle}u_k^{(n)}\big)^2 - \frac{9q}{2}\big(f_k^{(n)}\big)^2 + 3\big(r_k^{(n)}\big)^2\right\}\Delta x \\ &\qquad \le LC_0^2\left(\frac{27r^2\Lambda^4}{-8q} - \frac{9q}{2} + 3\right)\Delta t\left(\Delta x^2 + \Delta t^2\right)^2. \end{aligned} \tag{7.21}$$

Through this evaluation and $\varepsilon^{(0)} = 0$ and $\varepsilon^{(1)} \le C_0^2 L\Delta t^4$, we obtain

$$\begin{aligned}\max\big(\varepsilon^{(n+1)},\varepsilon^{(n)}\big) &\le R\max\big(\varepsilon^{(n)},\varepsilon^{(n-1)}\big) + \mathrm{RHS}\,(7.21) \\ &\le R^n LC_0^2\Delta t^4 + \left(\sum_{s=0}^{n-1} R^s\right)\cdot \mathrm{RHS}\,(7.21), \end{aligned} \tag{7.22}$$

where

$$R \stackrel{\text{def}}{=} 1 + \left(3 + \frac{9p^2 + 135r^2\Lambda^4}{-2q}\right)\Delta t. \tag{7.23}$$

Finally, applying

$$1 < R^n \le \exp\left\{\left(3 + \frac{9p^2 + 135r^2\Lambda^4}{-2q}\right)T\right\} \tag{7.24}$$

to this inequality, we obtain the following theorem, showing that the order of $\|\text{error}\|_{L_2}$ is $O\left((\Delta x)^2 + (\Delta t)^2\right)$.

THEOREM 7.1. *When $u(x,\cdot) \in C^3[0,T]$ for any fixed x and $u(\cdot,t) \in C^6[0,L]$ for any fixed t and the time mesh size Δt satisfies the condition (7.14), the error of the numerical solutions is bounded as follows:*

$$\left\{\sum_{k=0}^{N}{}'' \left(u_k^{(n)} - U_k^{(n)}\right)^2 \Delta x\right\}^{1/2} \le C_1 e^{C_2 T}(\Delta x^2 + \Delta t^2), \tag{7.25}$$

where

$$C_1 \stackrel{\text{def}}{=} C_0 \left\{\left(1 + \frac{3q^2 - 2q + (9/4)r^2\Lambda^4}{3p^2 - 2q + 45r^2\Lambda^4}\right)\cdot L\right\}^{1/2}, \tag{7.26}$$

$$C_2 \stackrel{\text{def}}{=} \frac{3}{2} + \frac{9p^2 + 135r^2\Lambda^4}{-4q}. \tag{7.27}$$

Comparing the solvability condition (6.7) and the converging condition (7.14), we see the inequality

$$\text{RHS}\,(7.14) \le \text{RHS}\,(6.7). \tag{7.28}$$

This implies that when $\Delta t \le \text{RHS}\,(7.14)$ there exists a unique numerical solution converging with order $O\left((\Delta x)^2 + (\Delta t)^2\right)$.

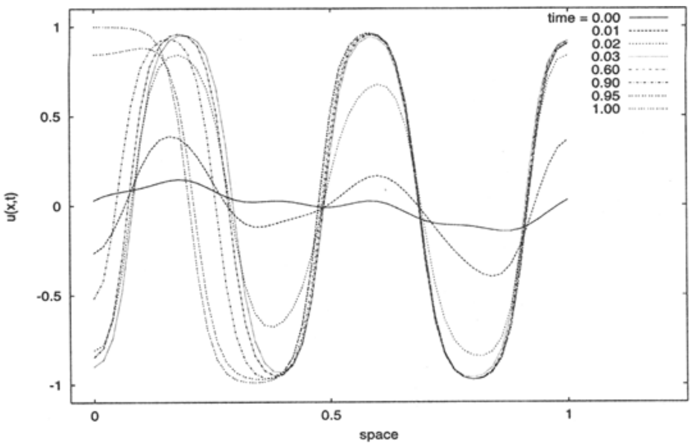
8. Examples of Numerical Solution

The purpose of this section is to demonstrate through numerical experiments that the proposed difference scheme is stable and gives reasonable numerical solutions.

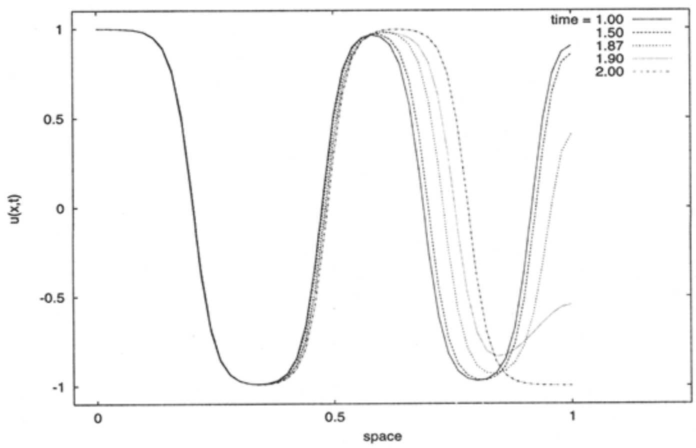
Figure 1 shows a numerical result for the Cahn-Hilliard equation with $p = -1.0$, $q = -0.001$ and $r = 1.0$ obtained by the proposed scheme with $\Delta x = 1/50$ and $\Delta t = 1/1000$. The initial state is

$$u(x,0) = 0.1\sin(2\pi x) + 0.01\cos(4\pi x) + 0.06\sin(4\pi x) + 0.02\cos(10\pi x). \tag{8.1}$$

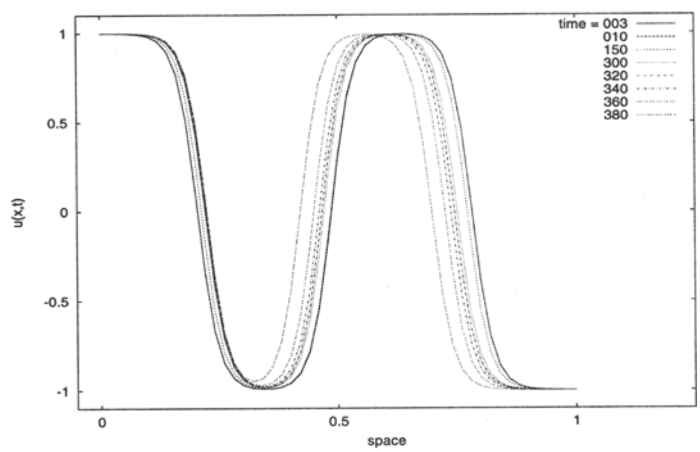
We can see that the final numerical solutions of Fig. 1 correspond exactly to the monotone solution that is the global minimizer of the total free energy [3]. The numerical solutions in Fig. 1 stand in virtual agreement with the results in [13] which were obtained by an explicit finite difference scheme and in [11] by a nonlinear implicit finite difference scheme. However, we must set Δt as small as



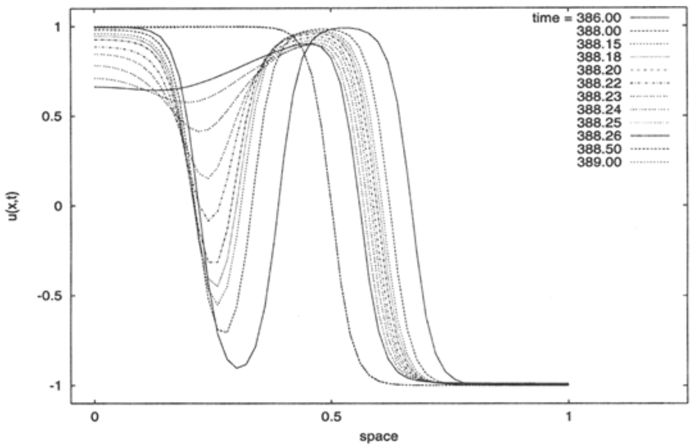
$t = 0.0 \cdots 1.0$



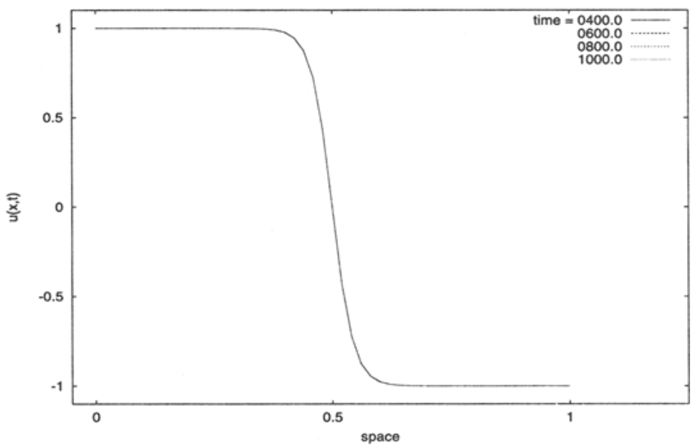
$t = 1.0 \cdots 2.0$



$t = 3.0 \cdots 380.0$



$t = 386.0 \cdots 389.0$



$t = 400.0 \cdots 1000.0$

Fig. 1. Numerical solution to the Cahn-Hilliard equation ($p = -1.0$, $q = -0.001$, $r = 1.0$) obtained by the proposed scheme (3.1)–(3.3) with $\Delta x = 1/50$ and $\Delta t = 1/1000$. The initial state is (8.1).

$5.9360656 \cdots \times 10^{-7} \cong 1/1685000$ in the scheme of the preceding paper [13], whereas we obtained a stable solution with a mesh size as large as $\Delta t = 1/1000$ by utilizing the present scheme. We used the same mesh size $\Delta t = 1/1000$ to the scheme in [11], but the computation time was much larger because the preceding scheme is implicit with nonlinearity.

Figure 2 shows the discrete total energy of numerical solution $\sum_{k=0}^{N}{}'' \, G_d(U^{(n+1)}, U^{(n)})_k \Delta x$ for the solution in Fig. 1. This graph shows that the decrease of total energy (4.6) is preserved numerically. Figure 3 shows the discrete total mass of numerical solution $\sum_{k=0}^{N}{}'' \, U_k^{(n)} \Delta x$ for the solution in Fig. 1. This graph shows that the conservation of the total mass (4.5) is preserved numerically.

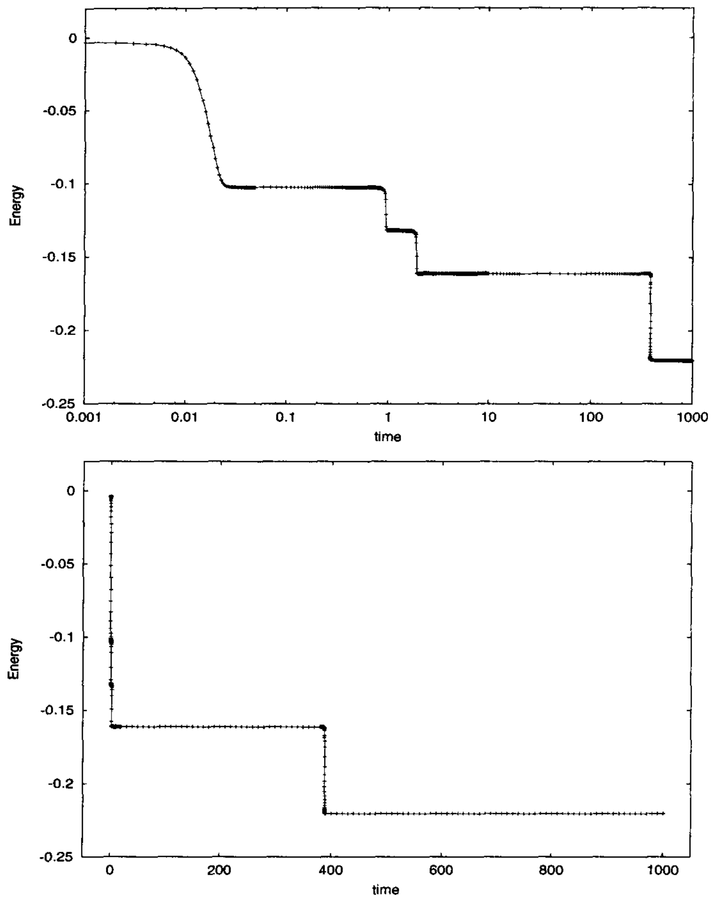


Fig. 2. The discrete total energy of the numerical solution in Fig. 1. The first one is log-scaled and the second is linear-scaled.

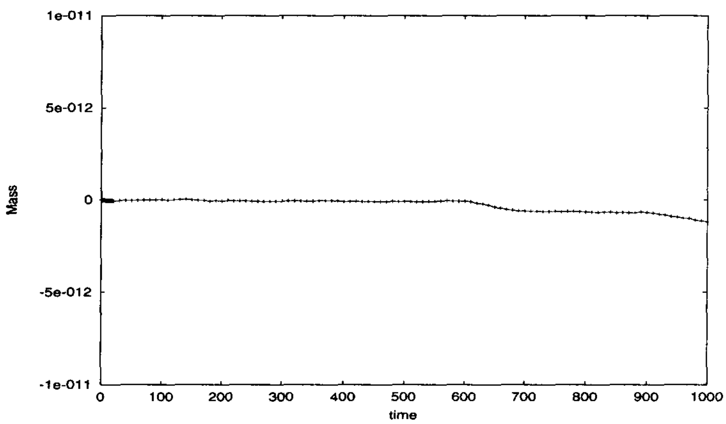


Fig. 3. The discrete total mass of the numerical solution in Fig. 1.

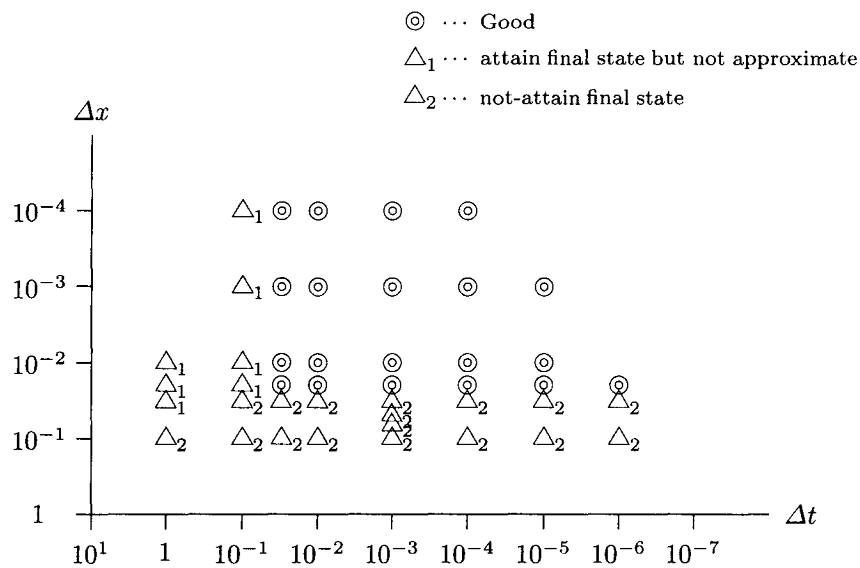


Fig. 4. Results of numerical solution to the Cahn-Hilliard equation ($p = -1.0$, $q = -0.001$, $r = 1.0$) obtained by the proposed scheme (3.1)–(3.3) with various Δx and Δt.

Figure 4 shows the results of numerical solution to the Cahn-Hilliard equation with $p = -1.0$, $q = -0.001$, $r = 1.0$ obtained by the proposed scheme with various Δx and Δt. The initial states are (8.1). The "Good" result means that the numerical solution has the following characteristics:

- Stable evolution,
- Attainment to the final state of which the shape is monotone,
- Close approximation to the solution of the Cahn-Hilliard equation,
- Decrease of the total energy as (4.6),
- Conservation of the total mass as (4.5).

We are able to estimate whether the obtained numerical solution sufficiently approximates the solution of the Cahn-Hilliard equation or not on the basis of the existing studies of numerical solutions of the equation as mentioned in §1. The "attain final state but not approximate" result means that the numerical solution attains the final state but the evolution does not approximate the solution of Cahn-Hilliard equation. The "not-attain final state" result is a case worse than the above ones, which means that the numerical solution is trapped by local-minimum of energy function and does not reach a monotone solution.

We must note that no numerical solution is observed to be unstable with these parameters. This confirms the remark of the Theorem 5.3 which means the proposed scheme is unconditionally stable.

With these parameter values, the bound of solution is estimated as

$$\Lambda = \sup_{x,t} \max\left(|u|, |U_k^{(n)}|\right) \le \sqrt{\frac{-p}{r}} = 1, \tag{8.2}$$

and the condition for the unique solvability of (6.7) is evaluated as

$$\Delta t < \frac{-4q}{r^2} = 0.004. \tag{8.3}$$

9. Conclusion

We proposed a new finite difference scheme to obtain numerical solutions to the Cahn-Hilliard equation. The proposed scheme is stable, L_2-convergent and linear and has a unique solution. The simultaneous realization of linearity and stability makes the proposed scheme substantially superior to other known schemes. The numerical solutions should be obtained by solving simultaneous linear equations per iteration. However, the computation time is proportional to N because of the bandedness of the coefficient matrix. Numerical examples demonstrated that the proposed scheme is very effective.

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