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

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Abstract

We propose a stable, convergent, conservative and linear finite difference scheme to solve numerically the Cahn-Hilliard equation. Its most essential property is to realize both linearity and stability. In addition to them, we show the uniqueness, existence and the convergence of the solution to the scheme. Numerical examples demonstrate the effectiveness of the proposed scheme.

Keywords: Finite difference method, Linear scheme, Decrease of Energy, Conservation of Mass, Cahn-Hilliard equation.

AMS subject classification: 35K55, 58J70, 65M06

1 Introduction

The Cahn-Hilliard equation [2]

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{\delta G}{\delta u}\right), \qquad x \in (0, L) \subset \mathbf{R}, 0 < t \tag{1}$$

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

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

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

$$\left.\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right|_{x=0} = \left.\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right|_{x=L} = 0, \tag{4}$$

i.e.,

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=L} = 0, \tag{5}$$

$$\left.\frac{\partial^3 u}{\partial x^3}\right|_{x=0} = \left.\frac{\partial^3 u}{\partial x^3}\right|_{x=L} = 0. \tag{6}$$

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The functional G means a local free energy called the Ginzburg–Landau free energy. The notation $\dfrac{\delta G}{\delta u}$ defined by (2) is consistent with the variational derivative of

$$G(u(x,t)) = \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(\frac{\partial u}{\partial x})^2 \tag{7}$$

with respect to $u(x,t)$. In fact, the relation between G of (7) and $\dfrac{\delta G}{\delta u}$ of (2)

$$\lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{\int_0^L G(u+\epsilon v)\,dx - \int_0^L G(u)\,dx\right\} = \int_0^L v\frac{\delta G}{\delta u}\,dx \tag{8}$$

is derived through integration by parts under the boundary condition (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

$$H_E^2(\Omega) \equiv \left\{f \in H^2(\Omega);\ \frac{\partial f}{\partial \nu} = 0 \text{ on } \partial\Omega\right\}, \tag{9}$$

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.

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 also stable, 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 condition for Δt and Δx. 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:

$$\mathrm{o}^{\langle 0\rangle} \overset{\text{def}}{=} 1, \tag{10}$$

$$\mathrm{o}^{\langle 1\rangle} \overset{\text{def}}{=} \frac{1}{2}(\mathrm{o}^{+}+\mathrm{o}^{-}), \tag{11}$$

$$\mathrm{o}^{\langle 2\rangle} \overset{\text{def}}{=} \mathrm{o}^{+}\mathrm{o}^{-}, \tag{12}$$

$$\mathrm{o}^{\langle 2m+1\rangle} \overset{\text{def}}{=} \mathrm{o}^{\langle 1\rangle}\mathrm{o}^{\langle 2m\rangle}, \qquad m \geq 1, \tag{13}$$

$$\mathrm{o}^{\langle 2m+2\rangle} \overset{\text{def}}{=} \mathrm{o}^{\langle 2\rangle}\mathrm{o}^{\langle 2m\rangle}, \qquad m \geq 1. \tag{14}$$

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.

$$s_j^{\pm} f(j) \overset{\text{def}}{=} f(j\pm 1), \tag{15}$$

$$\mu_j^{\pm} \overset{\text{def}}{=} \frac{s_j^{\pm}+1}{2}, \tag{16}$$

$$\delta_j^{\pm} \overset{\text{def}}{=} \frac{s_j^{\pm}-1}{\pm\Delta j}, \tag{17}$$

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

$$\Delta n \overset{\text{def}}{=} \Delta t, \tag{18}$$

$$\Delta k \overset{\text{def}}{=} \Delta x. \tag{19}$$

The generic rules (10)-(14) applied to $\mathrm{o}^{\pm} = s^{\pm}, \mu^{\pm}$ 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

$$\sum_{k=0}^{N}{}'' f_k \overset{\text{def}}{=} \frac{1}{2}f_0 + \sum_{k=1}^{N-1} f_k + \frac{1}{2}f_N. \tag{20}$$

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

$$\sum_{k=0}^{N}{}'' \left(\delta_k^{\langle h\rangle} f_k\right)\Delta x = \left[\mu_k^{\langle h \bmod 2\rangle}\delta_k^{\langle h-1\rangle} f_k\right]_{k=0}^{N}, \tag{21}$$

where

$$[f_k]_{k=0}^{N} \overset{\text{def}}{=} f_N - f_0. \tag{22}$$

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

$$\sum_{k=0}^{N}{}'' f_k\,(\delta_k^{+} g_k)\,\Delta x + \sum_{k=0}^{N}{}'' (\delta_k^{-} f_k)\, g_k \Delta x = \left[\frac{f_k\,(s_k^{+} g_k) + (s_k^{-} f_k)\, g_k}{2}\right]_{k=0}^{N}. \tag{23}$$

3 The Proposed Scheme

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

$$\frac{U_k^{(1)} - u_0(k\Delta x)}{\Delta t} = \frac{\partial^2}{\partial x^2}\left(\frac{\delta G(u_0(x))}{\delta u}\right)\bigg|_{x=k\Delta x}, \tag{24}$$

$$\delta_n^{\langle 1\rangle} U_k^{(n)} = \delta_k^{\langle 2\rangle} V_k^{(n)}, \quad n = 1, 2, \cdots, \tag{25}$$

$$V_k^{(n)} = pU_k^{(n)} + r\left(s_n^{\langle 1\rangle} U_k^{(n)}\right)\left(U_k^{(n)}\right)^2 + q\, \delta_k^{\langle 2\rangle}\left(s_n^{\langle 1\rangle} U_k^{(n)}\right), \tag{26}$$

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

$$U_{-1}^{(n)} = U_1^{(n)}, \qquad U_{N+1}^{(n)} = U_{N-1}^{(n)}, \tag{27}$$

$$U_{-2}^{(n)} = U_2^{(n)}, \qquad U_{N+2}^{(n)} = U_{N-2}^{(n)}, \tag{28}$$

for $n = 0, 1, 2, \ldots$. These conditions correspond (5) and (6). Note that these conditions satisfy

$$\left.\delta_k^{\langle 1\rangle} U_k^{(n)}\right|_{k=0} = \left.\delta_k^{\langle 1\rangle} U_k^{(n)}\right|_{k=N} = 0, \tag{29}$$

$$\left.\delta_k^{\langle 1\rangle} V_k^{(n)}\right|_{k=0} = \left.\delta_k^{\langle 1\rangle} V_k^{(n)}\right|_{k=N} = 0, \tag{30}$$

which correspond (3) and (4).

From the concrete form of the proposed scheme (24),(25) and (26), it is easy to understand the scheme is linear for the new time step.

The proposed scheme is implicit in that we should 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 (58), is sparse.

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,

$$\int_0^L u(x,t)\, dx = \int_0^L u(x,0)\, dx, \tag{31}$$

$$\frac{d}{dt}\int_0^L G(u(x,t))\, dx \leq 0. \tag{32}$$

We call (31) the conservation of mass and (32) the decrease of the total energy. The conservation of mass (31) can be shown easily as follows :

$$\frac{d}{dt}\int_0^L u(x,t)\, dx = \int_0^L \frac{\partial u(x,t)}{\partial t}\, dx = \int_0^L \frac{\partial^2}{\partial x^2}\frac{\delta G}{\delta u}\, dx = \left[\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right]_{x=0}^L = 0, \tag{33}$$

in which the boundary condition (4) is used. The decrease of the total energy (32) can be shown similarly under same condition:

$$\frac{d}{dt}\int_0^L G(u(x,t))\, dx = \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\, dx = -\int_0^L \left\{\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right\}^2 dx \leq 0. \tag{34}$$

The main purpose of this section is to show that the proposed scheme (24)-(26) has properties corresponding respectively to (31) and (32), i.e.,

$$\sum_{k=0}^{N}{}'' U_k^{(n)}\Delta x = \begin{cases} \displaystyle\sum_{k=0}^{N}{}'' U_k^{(0)}\Delta x, & : \ n \text{ is even} \\ \displaystyle\sum_{k=0}^{N}{}'' U_k^{(1)}\Delta x, & : \ n \text{ is odd} \end{cases} \tag{35}$$

$$\sum_{k=0}^{N}{}'' G_d\left(U^{(n+1)}, U^{(n)}\right)_k \Delta x - \sum_{k=0}^{N}{}'' G_d\left(U^{(n)}, U^{(n-1)}\right)_k \Delta x \leq 0, \tag{36}$$

where

$$G_d(f,g)_k \stackrel{\text{def}}{=} \frac{1}{2}pf_kg_k + \frac{1}{4}r\,(f_k)^2\,(g_k)^2 - \frac{1}{2}q\left(\frac{(\delta_k^+ f_k)^2 + (\delta_k^- f_k)^2 + (\delta_k^+ g_k)^2 + (\delta_k^- g_k)^2}{4}\right) \tag{37}$$

is the discrete local free energy defined for a pair of vectors $f = \{f_k\}, g = \{g_k\}$. We call (35) the discrete conservation of mass and (36) the discrete decrease of the total energy. The discrete conservation of mass (35) can be shown as

$$\begin{aligned} \frac{1}{2\Delta t}\left\{\sum_{k=0}^{N}{}'' \,U_k^{(n+1)}\Delta x - \sum_{k=0}^{N}{}'' \,U_k^{(n-1)}\Delta x\right\} &= \sum_{k=0}^{N}{}'' \left\{\delta_n^{\langle 1\rangle} U_k^{(n)}\right\}\Delta x \\ &= \sum_{k=0}^{N}{}'' \left\{\delta_k^{\langle 2\rangle} V_k^{(n)}\right\}\Delta x \\ &= \left[\delta_k^{\langle 1\rangle} V_k^{(n)}\right]_{k=0}^{N} \\ &= 0 \end{aligned} \tag{38}$$

because of (21) and the boundary condition (30). The decrease of the discrete total energy (36) can be shown as

$$\begin{aligned} &\frac{1}{\Delta t}\left\{\sum_{k=0}^{N}{}'' \,G_d\left(U_k^{(n+1)}, U_k^{(n)}\right)_k \Delta x - \sum_{k=0}^{N}{}'' \,G_d\left(U_k^{(n)}, U_k^{(n-1)}\right)_k \Delta x\right\} \\ &\quad= \sum_{k=0}^{N}{}'' \left\{V_k^{(n)}\delta_n^{\langle 1\rangle} U_k^{(n)}\right\}\Delta x \\ &\quad= \sum_{k=0}^{N}{}'' \left\{V_k^{(n)}\delta_k^{\langle 2\rangle} V_k^{(n)}\right\}\Delta x \\ &\quad= \left[s_k^{\langle 1\rangle} V_k^{(n)}\cdot\delta_k^{\langle 1\rangle} V_k^{(n)}\right]_{k=0}^{N} - \frac{1}{2}\sum_{k=0}^{N}{}'' \left[\left\{\delta_k^+ V_k^{(n)}\right\}^2 + \left\{\delta_k^- V_k^{(n)}\right\}^2\right]\Delta x \\ &\quad= -\frac{1}{2}\sum_{k=0}^{N}{}'' \left[\left\{\delta_k^+ V_k^{(n)}\right\}^2 + \left\{\delta_k^- V_k^{(n)}\right\}^2\right]\Delta x \\ &\quad\le 0, \end{aligned} \tag{39}$$

because the relation between G_d and $V_k^{(n)}$ is given by

$$\begin{aligned} &\sum_{k=0}^{N}{}'' \,G_d\left(U^{(n+1)}, U^{(n)}\right)_k \Delta x - \sum_{k=0}^{N}{}'' \,G_d\left(U^{(n)}, U^{(n-1)}\right)_k \Delta x \\ &\quad= \sum_{k=0}^{N}{}'' \left\{V_k^{(n)}\left(\frac{U_k^{(n+1)} - U_k^{(n-1)}}{2}\right)\right\}\Delta x + \left[\partial V_k^{(n)}\right]_{k=0}^{N} \\ &\quad= \sum_{k=0}^{N}{}'' \left\{V_k^{(n)}\left(\frac{U_k^{(n+1)} - U_k^{(n-1)}}{2}\right)\right\}\Delta x, \end{aligned} \tag{40}$$

where

$$\begin{aligned} \partial V_k^{(n)} \stackrel{\text{def}}{=} \frac{-q}{8}\Big\{ &\delta_k^+\left(s_n^{\langle 1\rangle} U_k^{(n)}\right)\cdot s_k^+\left(U_k^{(n+1)} - U_k^{(n-1)}\right) \\ &+\delta_k^-\left(s_n^{\langle 1\rangle} U_k^{(n)}\right)\cdot s_k^-\left(U_k^{(n+1)} - U_k^{(n-1)}\right) \\ &+2\delta_k^{\langle 1\rangle}\left(s_n^{\langle 1\rangle} U_k^{(n)}\right)\cdot\left(U_k^{(n+1)} - U_k^{(n-1)}\right)\Big\}. \end{aligned} \tag{41}$$

The boundary terms in (39) and (40) vanish because of (27) and (30). It is noted that the summation by parts (23) is used repeatedly in (40).

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 1 *The solutions $U_k^{(n)}$, $n = 0, 1, \ldots$, of the scheme (24)-(26) under the boundary conditions (27), (28) satisfy:*

$$\sum_{k=0}^{N-1} (\delta_k^+ U_k^{(n)})^2 \Delta x \le \left(\frac{4}{-q}\right) \left\{ \sum_{k=0}^{N}{}'' \, G_d\left(U^{(1)}, U^{(0)}\right)_k \Delta x + \frac{p^2 L}{4r} \right\}. \tag{42}$$

Proof : Applying $(r/4)x^2 + (p/2)x \ge -p^2/4r$ to the discrete local free energy in (37) we obtain:

$$\begin{aligned} &\sum_{k=0}^{N}{}'' \, G_d\left(U^{(n+1)}, U^{(n)}\right)_k \Delta x \\ &\quad \ge \sum_{k=0}^{N}{}'' \left\{ -\frac{p^2}{4r} - \frac{q}{8}\left((\delta_k^+ U_k^{(n+1)})^2 + (\delta_k^- U_k^{(n+1)})^2 + (\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2 \right) \right\} \Delta x \\ &\quad \ge \sum_{k=0}^{N}{}'' \left\{ -\frac{p^2}{4r} - \frac{q}{8}\left((\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2 \right) \right\} \Delta x \\ &\quad = -\frac{p^2}{4r} L - \frac{q}{4} \sum_{k=0}^{N-1} (\delta_k^+ U_k^{(n)})^2 \Delta x, \end{aligned} \tag{43}$$

since

$$\sum_{k=0}^{N}{}'' \left\{ \left((\delta_k^+ U_k^{(n)})^2 + (\delta_k^- U_k^{(n)})^2 \right) \right\} \Delta x = 2 \sum_{k=0}^{N-1} (\delta_k^+ U_k^{(n)})^2 \Delta x \tag{44}$$

under the discrete boundary conditions (27), (28). The inequality (42) follows from the above inequality and the decrease of the total energy (36). □

LEMMA 2 *For any $f = \{f_k\}_{k=0}^N$ and $0 \le {}^\forall m \le N$, the following inequality is satisfied:*

$$\frac{1}{L}\left(f_m - \frac{M}{L}\right)^2 \le \sum_{k=0}^{N-1} \left(\delta_k^+ f_k\right)^2 \Delta x, \tag{45}$$

where

$$M \stackrel{\text{def}}{=} \sum_{k=0}^{N}{}'' \, f_k \Delta x. \tag{46}$$

Proof : For any m such that $0 \le m \le N$ we have

$$f_m L - M = \sum_{k=0}^{N}{}'' \, (f_m - f_k)\, \Delta x = \sum_{k=0}^{N}{}'' \, \gamma_{k,m}(f) \Delta x, \tag{47}$$

where

$$\gamma_{k,m}(f) \stackrel{\text{def}}{=} \begin{cases} \displaystyle\sum_{l=k}^{m-1} (\delta_l^+ f_l)\, \Delta x & : \quad k \le m, \\ \displaystyle -\sum_{l=m}^{k-1} (\delta_l^+ f_l)\, \Delta x & : \quad m < k. \end{cases} \tag{48}$$

This implies

$$\left| f_m - M/L \right| \le \sum_{k=0}^{N-1} \left| \delta_k^+ f_k \right| \Delta x, \tag{49}$$

since

$$\begin{aligned} \left| f_m L - M \right| &\le \sum_{k=0}^{N}{}'' \left| \gamma_{k,m}(f) \right| \Delta x, &(50)\\ \left| \gamma_{k,m}(f) \right| &\le \sum_{k=0}^{N-1} \left| \delta_k^+ f_k \right| \Delta x. &(51) \end{aligned}$$

Finally, applying the Schwartz inequality to (49) we obtain the inequality (45). □

Remark : The inequality (49) corresponds to the Poincare–Wirtinger inequality [1, p. 146]. □

Applying Lemma 2 to (42) we obtain the following theorem.

THEOREM **3** *The solutions $U_k^{(n)}$, $n = 1, 2, \ldots$, of the scheme (24)-(26) under the boundary conditions (27), (28) satisfy*

$$U_C^- - \Delta U \le U_k^{(n)} \le U_C^+ + \Delta U, \tag{52}$$

where

$$\begin{aligned} U_C^+ &\stackrel{\text{def}}{=} \frac{1}{L} \max\left(\sum_{k=0}^{N}{}'' U_k^{(0)} \Delta x, \sum_{k=0}^{N}{}'' U_k^{(1)} \Delta x \right), &(53)\\ U_C^- &\stackrel{\text{def}}{=} \frac{1}{L} \min\left(\sum_{k=0}^{N}{}'' U_k^{(0)} \Delta x, \sum_{k=0}^{N}{}'' U_k^{(1)} \Delta x \right), &(54)\\ \Delta U &\stackrel{\text{def}}{=} \left[\left(\frac{4L}{-q} \right) \left\{ \sum_{k=0}^{N}{}'' G_d \left(U^{(1)}, U^{(0)} \right)_k \Delta x + \frac{p^2 L}{4r} \right\} \right]^{1/2}. &(55) \end{aligned}$$

The inequality (52) implies that the proposed difference scheme (24)-(26) is stable for any time step n since the constants $U_C^{\pm}$, ΔU are determined by the initial state.

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 (25) has a unique solution under a certain condition on Δt and Δx.

The equation (24) has a unique solution without any condition. The equations (25), (26) can be rewritten as simultaneous linear equations

$$\begin{aligned} &\left\langle 1 - 2\Delta t \left[\frac{r}{2\Delta x^2} \left\{ \left(U_{k+1}^{(n)} \right)^2 s_k^+ - 2 \left(U_k^{(n)} \right)^2 + \left(U_{k-1}^{(n)} \right)^2 s_k^- \right\} + \frac{q}{2} \delta_k^{\langle 4 \rangle} \right] \right\rangle U_k^{(n+1)} \\ &\quad = 2\Delta t \delta_k^{\langle 2 \rangle} \left\{ p U_k^{(n)} + \frac{r}{2} \left(U_k^{(n)} \right)^2 U_k^{(n-1)} \right\} + \left(1 + \Delta t q \delta_k^{\langle 4 \rangle} \right) U_k^{(n-1)} \end{aligned} \tag{56}$$

Under the discrete boundary conditions (27), (28), the above simultaneous linear equations are written as

$$A\, U^{(n+1)} = w, \tag{57}$$

where A is an $(N+1)\times(N+1)$ matrix and $w=\{w_k\}_{k=0}^{N}$ is a vector with $w_k \overset{\text{def}}{=}$ RHS of (56). The elements $A_{ij}, (0\le i,j\le N)$ of the matrix A are

$$A_{ij} = \begin{cases} 1+a_i^{(n)} & : \quad i=j, i\neq 1, \\ b_j^{(n)} & : \quad i=j\pm 1, i\neq 0, i\neq N, \\ c & : \quad i=j\pm 2, i\neq 0, i\neq N, \\ 1+a_i^{(n)}+c & : \quad (i,j)=(1,1) \\ 2b_j^{(n)} & : \quad (i,j)=(0,1),(N,N-1), \\ 2c & : \quad (i,j)=(0,2),(N,N-2), \\ 0 & : \quad \text{otherwise,} \end{cases} \tag{58}$$

where

$$a_k^{(n)} \overset{\text{def}}{=} \Delta t\left\{\frac{2r}{\Delta x^2}\left(U_k^{(n)}\right)^2-\frac{6q}{\Delta x^4}\right\}, \qquad k=0,1,\ldots,N, \tag{59}$$

$$b_k^{(n)} \overset{\text{def}}{=} \Delta t\left\{-\frac{r}{\Delta x^2}\left(U_k^{(n)}\right)^2+\frac{4q}{\Delta x^4}\right\}, \qquad k=0,1,\ldots,N, \tag{60}$$

$$c \overset{\text{def}}{=} \frac{-q\Delta t}{\Delta x^4}. \tag{61}$$

We obtain the following theorem.

Theorem 4 *When*

$$\Delta t < \frac{\Delta x^4}{-4q+2r\Delta x^2\max\left\{\left(U_C^- -\Delta U\right)^2, \left(U_C^+ +\Delta U\right)^2\right\}} \tag{62}$$

the proposed scheme (24)-(26) has a unique solution.

Proof : From the Gerschgorin theorem (cf.[20, pp.132–135]) all eigenvalues of the matrix A are non-zero if

$$1+a_k^{(n)} > \left|b_{k-1}^{(n)}\right|+\left|b_{k+1}^{(n)}\right|+2\,|c|\,, \tag{63}$$

for $0\le {}^\forall k\le N$, where $b_{-1}^{(n)} \overset{\text{def}}{=} b_1^{(n)}$ and $b_{N+1}^{(n)} \overset{\text{def}}{=} b_{N-1}^{(n)}$. This inequality is equivalent the following inequality:

$$1 > -b_{k-1}^{(n)}-a_k^{(n)}-b_{k+1}^{(n)}+2c = \Delta t\left\{r\delta_k^{\langle 2\rangle}\left(U_k^{(n)}\right)^2-\frac{4q}{\Delta x^4}\right\}. \tag{64}$$

The condition (62) guarantees this above inequality, since

$$\begin{aligned} r\delta_k^{\langle 2\rangle}\left(U_k^{(n)}\right)^2 &\le \frac{2r}{\Delta x^2}\max_k\left(U_k^{(n)}\right)^2 \\ &\le \frac{2r}{\Delta x^2}\max\left\{\left(U_C^- -\Delta U\right)^2, \left(U_C^+ +\Delta U\right)^2\right\} \end{aligned} \tag{65}$$

from the Theorem 3. □

Remark : For the uniqueness and existence of the numerical solution in Theorem 4, the stability theorem (Theorem 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 (24)-(26) converges to the solution to the original equation (1)-(2).

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

$$v(x,t) \stackrel{\text{def}}{=} \frac{\delta G(u(x,t))}{\delta u}, \tag{66}$$

$$\tilde{u}_k^{(n)} \stackrel{\text{def}}{=} u_k^{(n)} - U_k^{(n)}, \tag{67}$$

$$\tilde{v}_k^{(n)} \stackrel{\text{def}}{=} v_k^{(n)} - V_k^{(n)}, \tag{68}$$

$$r_k^{(n)} \stackrel{\text{def}}{=} \delta_n^{\langle 1 \rangle} \tilde{u}_k^{(n)} - \delta_k^{\langle 2 \rangle} \tilde{v}_k^{(n)}, \tag{69}$$

$$h_k^{(n)} \stackrel{\text{def}}{=} \left(u_k^{(n)}\right)^3 - \left(\frac{U_k^{(n+1)} + U_k^{(n-1)}}{2}\right)\left(U_k^{(n)}\right)^2, \tag{70}$$

$$f_k^{(n)} \stackrel{\text{def}}{=} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x=k\Delta x, t=n\Delta t} - \delta_k^{\langle 2 \rangle}\left(\frac{u_k^{(n+1)} + u_k^{(n-1)}}{2}\right), \tag{71}$$

where $U_k^{(n)}$ is the solution of the proposed scheme (24)-(26), $V_k^{(n)}$ is defined in (26), $u(x,t)$ is the solution to the Cahn-Hilliard equation, $u_k^{(n)} \stackrel{\text{def}}{=} u(k\Delta x, n\Delta t)$, $v_k^{(n)} \stackrel{\text{def}}{=} v(k\Delta x, n\Delta t)$. We define an extension of u by

$$u(x,t) \stackrel{\text{def}}{=} \begin{cases} u(x - 2lL, t) & : \quad 2lL \le x \le (2l+1)L, \\ u(2lL - x, t) & : \quad (2l-1)L < x < 2lL, \end{cases} \tag{72}$$

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

Under the discrete boundary conditions (27), (28) and above definitions, we obtain the following inequality applying the summation by parts (23):

(73)

$$\begin{aligned} &\sum_{k=0}^{N}{}'' \left\{ s_n^{\langle 1 \rangle} \tilde{u}_k^{(n)} \cdot \delta_n^{\langle 1 \rangle} \tilde{u}_k^{(n)} + \frac{1}{-q}\left(\tilde{v}_k^{(n)}\right)^2 \right\} \Delta x \\ &= \sum_{k=0}^{N}{}''\left\{ s_n^{\langle 1 \rangle} \tilde{u}_k^{(n)} \cdot \left(\delta_k^{\langle 2 \rangle} \tilde{v}_k^{(n)} + r_k^{(n)}\right) + \frac{1}{-q}\tilde{v}_k^{(n)}\left(p\tilde{u}_k^{(n)} + rh_k^{(n)} + q\delta_k^{\langle 2 \rangle} s_n^{\langle 1 \rangle} \tilde{u}_k^{(n)} + qf_k^{(n)}\right)\right\} \Delta x \\ &= \sum_{k=0}^{N}{}''\left\{ s_n^{\langle 1 \rangle} \tilde{u}_k^{(n)} \cdot r_k^{(n)} + \frac{1}{-q}\tilde{v}_k^{(n)}\left(p\tilde{u}_k^{(n)} + rh_k^{(n)} + qf_k^{(n)}\right)\right\} \Delta x \\ &\le \sum_{k=0}^{N}{}''\left\{ \frac{1}{2}\left(s_n^{\langle 1 \rangle} \tilde{u}_k^{(n)}\right)^2 + \frac{1}{2}\left(r_k^{(n)}\right)^2 + \frac{1}{-q}\left\{\left(\tilde{v}_k^{(n)}\right)^2 + p^2\left(\tilde{u}_k^{(n)}\right)^2 + r^2\left(h_k^{(n)}\right)^2 + q^2\left(f_k^{(n)}\right)^2\right\}\right\} \Delta x. \end{aligned}$$

Cancelling $\frac{1}{-q}\left(\tilde{v}_k^{(n)}\right)^2$ from both sides and multiplying $4\Delta t$, we obtain

(74)

$$\begin{aligned} &\sum_{k=0}^{N}{}'' \left\{ \left(\tilde{u}_k^{(n+1)}\right)^2 - \left(\tilde{u}_k^{(n-1)}\right)^2 \right\} \Delta x \\ &\le \Delta t \sum_{k=0}^{N}{}''\left[\left(\tilde{u}_k^{(n+1)}\right)^2 + \left(\tilde{u}_k^{(n-1)}\right)^2 + 2\left(r_k^{(n)}\right)^2 + \frac{4}{-q}\left\{p^2\left(\tilde{u}_k^{(n)}\right)^2 + r^2\left(h_k^{(n)}\right)^2 + q^2\left(f_k^{(n)}\right)^2\right\}\right] \Delta x. \end{aligned}$$

Since the solution of the proposed scheme is bounded as shown in Theorem 3, we can evaluate $h_k^{(n)}$ when $u \in C^0([0,L] \times [0,T])$ as follows:

$$\left(h_k^{(n)}\right)^2 \le 3C_2^2 \left[\Delta t^4 \left(\delta_n^{\langle 2 \rangle} u_k^{(n)}\right)^2 + \frac{\left(\tilde{u}_k^{(n+1)}\right)^2 + \left(\tilde{u}_k^{(n-1)}\right)^2}{2} + 4\left(\tilde{u}_k^{(n)}\right)^2\right], \tag{75}$$

where

$$C_2 \stackrel{\mathrm{def}}{=} \max\left\{ \sup_{\substack{0\le x\le L\\ 0\le t\le T}} (u(x,t))^2, \left(U_C^- - \Delta U\right)^2, \left(U_C^+ + \Delta U\right)^2 \right\}, \tag{76}$$

and $T \geq (n+1)\Delta t$. Substituting the above estimate into the inequality (74) we obtain

$$\begin{aligned} &\left\{1 - \Delta t\left(1 + \frac{6r^2C_2^2}{-q}\right)\right\}\varepsilon^{(n+1)} \\ \le\ & \left\{1 + \Delta t\left(1 + \frac{6r^2C_2^2}{-q}\right)\right\}\varepsilon^{(n-1)} + \frac{4\Delta t}{-q}\left(p^2 + 12r^2C_2^2\right)\varepsilon^{(n)} \\ & + \Delta t \sum_{k=0}^{N}{}'' \left\{2\left(r_k^{(n)}\right)^2 - 4q\left(f_k^{(n)}\right)^2 + \frac{12r^2C_2^2}{-q}\Delta t^4\left(\delta_n^{\langle 2\rangle}u_k^{(n)}\right)^2\right\}\Delta x, \end{aligned} \tag{77}$$

where

$$\varepsilon^{(n)} \stackrel{\mathrm{def}}{=} \sum_{k=0}^{N}{}'' \left(\tilde{u}_k^{(n)}\right)^2 \Delta x. \tag{78}$$

For the time mesh size Δt satisfying

$$0 \le \Delta t \le \frac{1}{3}\left(\frac{1}{1 + \frac{6r^2C_2^2}{-q}}\right), \tag{79}$$

the inequality (77) implies

$$\begin{aligned} &\varepsilon^{(n+1)} \\ \le\ & \left\{1 + 3\Delta t\left(1 + \frac{6r^2C_2^2}{-q}\right)\right\}\varepsilon^{(n-1)} + \frac{6\Delta t}{-q}\left(p^2 + 12r^2C_2^2\right)\varepsilon^{(n)} \\ & + \Delta t \sum_{k=0}^{N}{}'' \left\{3\left(r_k^{(n)}\right)^2 - 6q\left(f_k^{(n)}\right)^2 + \frac{18r^2C_2^2}{-q}\Delta t^4\left(\delta_n^{\langle 2\rangle}u_k^{(n)}\right)^2\right\}\Delta x. \end{aligned} \tag{80}$$

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 there is a constant $C_4 > 0$ such that

$$\left|r_k^{(n)}\right| \le C_4\left((\Delta x)^2 + (\Delta t)^2\right), \tag{81}$$

$$\left|f_k^{(n)}\right| \le C_4\left((\Delta x)^2 + (\Delta t)^2\right), \tag{82}$$

$$\left|\delta_n^{\langle 2\rangle}u_k^{(n)}\right| \le C_4, \tag{83}$$

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

$$\begin{aligned} &\Delta t \sum_{k=0}^{N}{}'' \left\{3\left(r_k^{(n)}\right)^2 - 6q\left(f_k^{(n)}\right)^2 + \frac{18r^2C_2^2}{-q}\Delta t^4\left(\delta_n^{\langle 2\rangle}u_k^{(n)}\right)^2\right\}\Delta x \\ &\quad \le LC_4^2\left(3 - 6q + \frac{18r^2C_2^2}{-q}\right)\Delta t\left(\Delta x^2 + \Delta t^2\right)^2. \end{aligned} \tag{84}$$

Through this evaluation and $\varepsilon^{(0)} = 0$ and $\varepsilon^{(1)} \le C_4^2 L\Delta t^4$, we obtain

$$\begin{aligned} \max\left(\varepsilon^{(n+1)}, \varepsilon^{(n)}\right) &\le R\max\left(\varepsilon^{(n)}, \varepsilon^{(n-1)}\right) + C_5 \\ &\le R^n LC_4^2\Delta t^4 + \left(\sum_{s=0}^{n-1} R^s\right)C_5, \end{aligned} \tag{85}$$

where $C_5 \stackrel{\text{def}}{=}$ RHS of (84) and

$$R \stackrel{\text{def}}{=} 1 + \left(3 + \frac{6p^2 + 90r^2 C_2^2}{-q} \right) \Delta t. \tag{86}$$

Finally, applying

$$1 < R^n \le \exp\left\{ \left(3 + \frac{6p^2 + 90r^2 C_2^2}{-q} \right) T \right\} \tag{87}$$

to this inequality, we obtain the following theorem.

THEOREM **5** *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 (79), the error of the numerical solutions is bounded as follows:*

$$\left\{ \sum_{k=0}^{N}{}'' \left(u_k^{(n)} - U_k^{(n)} \right)^2 \Delta x \right\}^{1/2} \le C_6 e^{C_7 T} \sqrt{T} \left(\Delta x^2 + \Delta t^2 \right), \tag{88}$$

where

$$C_6 \stackrel{\text{def}}{=} (C_4)^2 \left\{ \left(4 - 6q + \frac{18r^2 C_2^2}{-q} \right) L \right\}^{1/2}, \tag{89}$$

$$C_7 \stackrel{\text{def}}{=} \frac{3}{2} + \frac{3p^2 + 45r^2 C_2^2}{-q}. \tag{90}$$

This theorem implies that the order of $\|\text{error}\|_{L_2}$ is $O\left((\Delta x)^2 + (\Delta t)^2 \right)$.

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

$$u(x, 0) = 0.1 \sin(2\pi x) + 0.01 \cos(4\pi x) + 0.06 \sin(4\pi x) + 0.02 \cos(10\pi x). \tag{91}$$

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 $5.9360656 \cdots \times 10^{-7} \cong 1/1685000$ 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 calculation time was much larger because the preceding scheme is implicit with nonlinearity.

Figure 2 shows the total discrete energy of numerical solution $\sum_{k=0}^{N}{}'' G_d(U^{(n+1)}, U^{(n)})_k \Delta x$ in Fig.1. This graph shows that the decrease of the total energy (36) is preserved numerically. Figure 3 shows the total discrete mass of numerical solution $\sum_{k=0}^{N}{}'' U_k^{(n)} \Delta x$ in Fig.1. This graph shows that the conservation of the total mass (35) is preserved numerically.

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 both of linearity and stability makes that 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 sparsity of the coefficient matrix. Numerical examples demonstrated that the proposed scheme is very effective.

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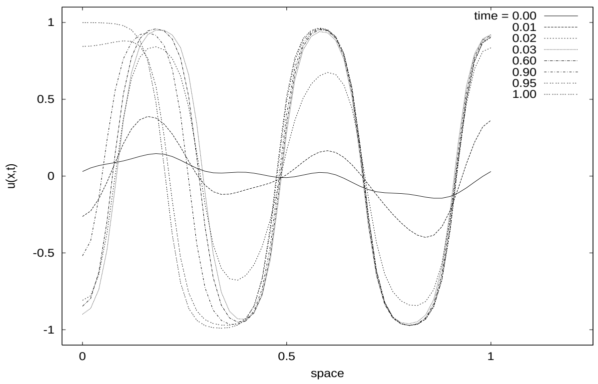
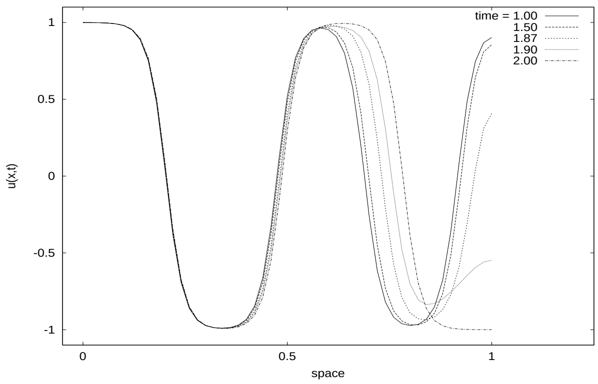
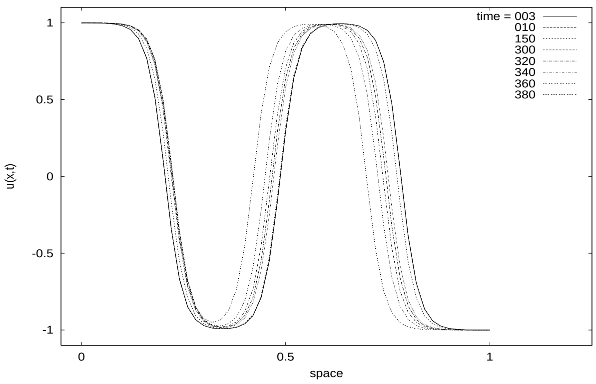


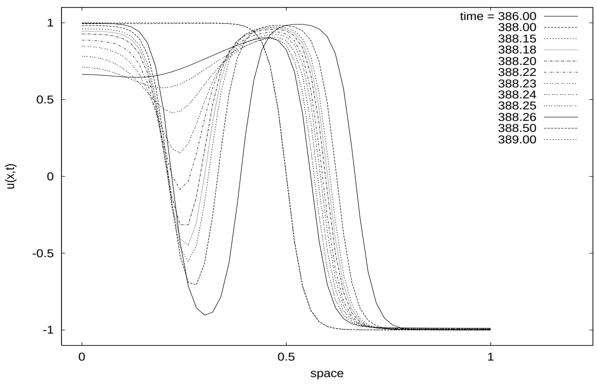
$t = 0.0 \cdots 1.0$



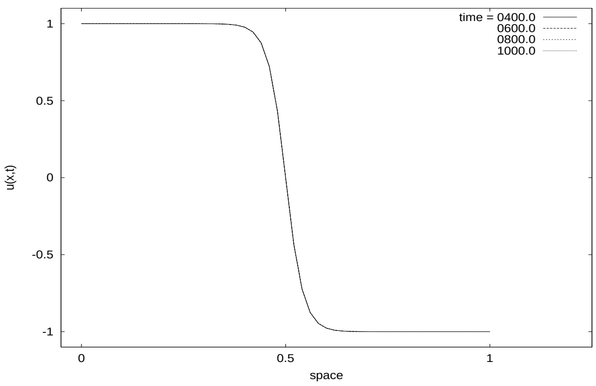
$t = 1.0 \cdots 2.0$



$t = 3.0 \cdots 380.0$



$t = 386.0 \cdots 389.0$



$t = 400.0 \cdots 1000.0$

Figure 1: Numerical solution to the Cahn-Hilliard equation ($p = -1.0$, $q = -0.001$, $r = 1.0$) obtained by the proposed scheme (24)-(26) with $\Delta x = 1/50$ and $\Delta t = 1/1000$. The initial state is (91).

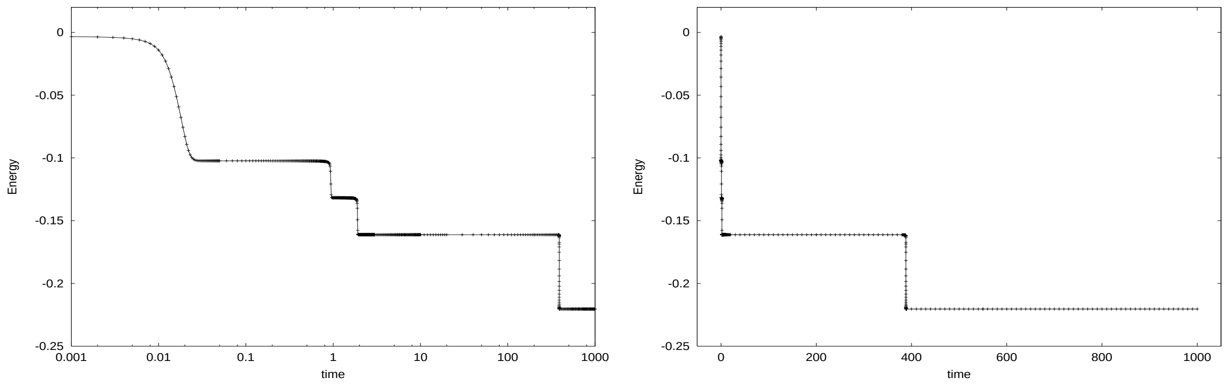


Figure 2: The discrete total energy of the numerical solution in Fig.1. The first one is log-scaled and the second is linear-scaled.

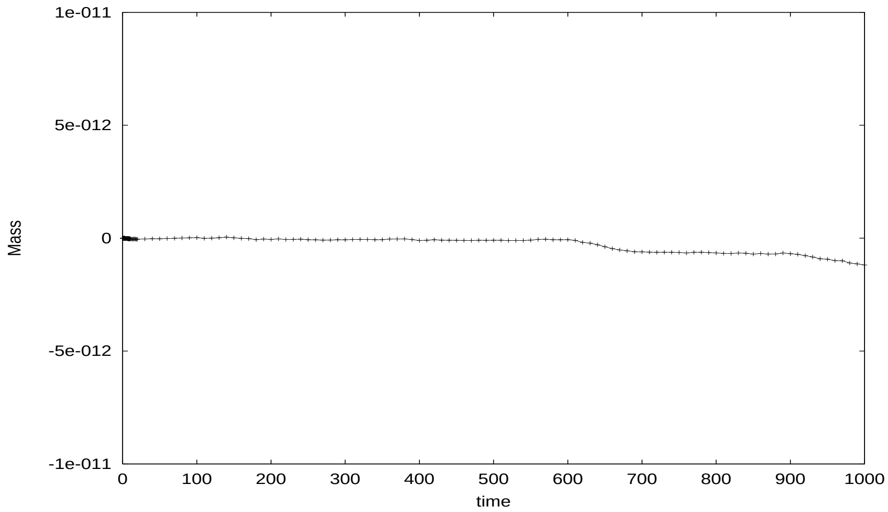


Figure 3: The discrete total mass of the numerical solution in Fig.1 .

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