CONVERGENCE ANALYSIS OF THE ENERGY-STABLE NUMERICAL SCHEMES FOR THE CAHN-HILLIARD EQUATION

by

Xiao-Rong KANG, Yan-Mei WU, and Ke-Long CHENG *

School of Science, Southwest University of Science and Technology, Mianyang, China

Original scientific paper
https://doi.org/10.2298/TSCI2202037K

In this paper we present a second order numerical scheme for the Cahn-Hilliard equation, with a Fourier pseudo-spectral approximation in space. An additional Douglas-Dupont regularization term is introduced, which ensures the energy stability. The bound of numerical solution in H_h^2 *and* ℓ^∞ *norms are obtained at a theoretical level. Moreover, for the global nature of the pseudo-spectral method, we propose a linear iteration algorithm to solve the non-linear system, due to the implicit treatment for the non-linear term. Some numerical simulations verify the efficiency of iteration algorithm.*

Key words: *Cahn-Hilliard equation, energy stability scheme, convergence, linear iteration*

Introduction

The Cahn-Hilliard (CH) equation [1], which models spinodal decomposition and phase separation in a binary alloy, is one of the best known gradient flow type models in mathematical physics. For any $\phi \in H^1(\Omega)$, the energy is given by:

$$E(\phi) = \int_\Omega \left(\frac{1}{4}\phi^4 - \frac{1}{2}\phi^2 + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right) \mathrm{d}x \tag{1}$$

where ε is a positive constant that dictates the interface width and the CH equation can be viewed as the H^{-1}conserved gradient flow of the energy functional (1):

$$\phi_t = \Delta\mu, \quad \text{with} \;\; \mu := \delta_\phi E = \phi^3 - \phi - \varepsilon^2 \Delta\phi \tag{2}$$

Here we consider dimension two and take the spatial domain Ω to be the usual 2π-periodic torus. Subsequently, the energy dissipation law follows from an inner product with (2) by μ. Meanwhile, the equation also is mass conservative.

The analysis for the CH equation turns out to be quite challenging, since it is a fourth-order, non-linear parabolic type PDE. Many numerical works have reported interesting computational results for CH equation [2-7]. Among these results, one usually investigates the semi-implicit or fully implicit numerical schemes because of the difficulties introduced by the combination of non-linearity and stiffness. Meanwhile, of these works, with a cut-off of the double-well energy and artificial stabilization term, Wu *et al.* [2] proposed a linear second-

* Corresponding author, e-mail: zhengkelong@swust.edu.cn

order scheme for CH type equations and diffuse interface tumor models. Guillen-Gonzalez and Tierra [3] presented a linearized second-order scheme with an alternate variable. Based on the modified version of the Crank-Nicolson discretization, a convex splitting finite difference scheme for CH equation was also reported in [4].

Recently, spectral and pseudo-spectral schemes are often considered when high-resolution solvers are sought for the CH equation. For the periodic boundary condition, the Fourier method is a natural choice to obtain the optimal spatial accuracy. For example, a convex splitting Fourier collocation spectral scheme with an implicit treatment of non-linear terms has been discussed in [8].

In this paper, a semi-implicit Fourier pseudo-spectral numerical scheme for CH equation with the BDF three-point stencil in the temporal approximation is discussed. The results show theoretically and numerically that the proposed scheme can achieve the best stability performance. In addition, the energy stability of the proposed scheme also gives a uniform H^1 bound at a discrete level. As a result, $\ell^\infty(0, T; H^2)$ and $\ell^\infty(0, T; L^\infty)$ estimates of the numerical solution are proved. Similar to the linear iteration algorithm reported in [8] for the modified Crank-Nicolson scheme, the linear iteration solver is employed again for this scheme.

Notations

For simplicity of presentation, we use a square domain, *i.e.*, $L = 1$ and a uniform mesh size $h_x = h_y = h$, $N_x = N_y = N$. We will assume that $N = 2K + 1$ is always odd. All the variables are evaluated at the regular numerical grid (x_i, y_j), with $x_i = ih$, $y_i = jh$, $0 \le I, j \le N$.

For a periodic function f over the given 2-D numerical grid, we define the grid function space:

$$G_N := \{ f : Z^2 \to R \mid f \text{ is periodic} \}$$

As for definitions and properties of ∇_N and Δ_N used in the next section, see the details in [8].

The spectral approximations to the ℓ^2 inner product and norm are introduced as:

$$\| f \|_2 = \sqrt{< f, f >}, \qquad < f, g >= h^2 \sum_{i,j=0}^{N-1} f_{i,j} g_{i,j}$$

and the l^∞ and $l^p, 1 \le p < \infty$ norms for a grid function:

$$\| f \|_\infty := \max_{0 \le i,j \le N-1} | f_{i,j} |, \qquad \| f \|_p := (h^2 \sum_{i,j=0}^{N-1} | f_{i,j} |^p)^{1/p} \tag{3}$$

To obtain a pseudo-spectral approximation at a given set of points, an interpolation operator I_N should be introduced. Given a uniform numerical grid with $2N + 1$ points in each dimension and a discrete vector function f, where each point is denoted by (x_i, y_j) and the corresponding function value is given by $f_{i,j}$, the interpolation of the function is:

$$(I_N f)(x, y) = \sum_{l,m=-N}^{N} (\hat{f}_c^N)_{l,m} \exp[2\pi i(lx + my)] \tag{4}$$

where the $(2N + 1)^2$ pseudo-spectral coefficients $(\hat{f}_c^N)_{l,m}$ are given by the interpolation condition $f_{i,j} = (I_N f)(x_i, y_j)$.

The following lemma enables us to obtain an H^m bound of the interpolation of the non-linear term; the detailed proof can be found in [9].

Lemma 1. Suppose that m and K are non-negative integers, and $N = 2K + 1$. For any $\phi \in P_{nK}$ (with trigonometric polynomial up to degree nK) in R^d, we have the estimate:

$$\|I_N\phi\|_{H^r} \le (\sqrt{n})^d \|\phi\|_{H^r} \tag{5}$$

for any non-negative integer r.

The fully discrete numerical scheme

By the Fourier pseudo-spectral discretization in space, the second order accurate in time backward differentiation formula (BDF) type numerical scheme can be formulated as follows: for $m \ge 1$, given φ^m, $\varphi^{m-1} \in G_N$, find $\varphi^{m+1} \in G_N$ such that:

$$\frac{3\phi^{m+1} - 4\phi^m + \phi^{m-1}}{2s} = \Delta_N[(\phi^{m+1})^3 - (2\phi^m - \phi^{m-1}) - \varepsilon^2\Delta_N\phi^{m+1}] -$$
$$-As(-\Delta_N)^2(\phi^{m+1} - \phi^m) + B\Delta_N(\phi^{m+1} - 2\phi^m + \phi^{m-1}) \tag{6}$$

where $s = T/M$.

To investigate the energy stability of eq. (6), we introduce the following modified discrete energy:

$$E_N(\phi,\varphi) = \frac{1}{4}\|\phi\|_4^4 - \frac{1}{2}\|\phi\|_2^2 + \frac{\varepsilon^2}{2}\|\nabla_N\phi\|_2^2 + \frac{1}{4s}\|\phi-\varphi\|_{-1,N}^2 + \frac{B+1}{2}\|\phi\|_2^2 \tag{7}$$

The analogue results for the energy-decay property of eq. (6) can follow by an similar argument with suitable modification in [8]; the details are skipped for simplicity.

Theorem 1. For any $B \ge 0$ and given $\phi^m, \phi^{m-1} \in G_N$, the numerical eq. (6) is unconditionally energy stable, *i.e.*, if $A \ge 1/16$, we have:

$$E_N(\phi^{m+1},\phi^m) \le E_N(\phi^m,\phi^{m-1}) \le \ldots \le E_N(\phi^0,\phi^{-1}) \le C_0 \tag{8}$$

Maximum estimate of the numerical solutions

Lemma 2. Suppose that $\phi^m \in G_N, m = 1,2,\ldots,M$ are the unique solutions to eq. (6). Then, we have the following estimates:

$$\left\|\phi^m\right\|_4 \le C_1, \quad \left\|\phi^m\right\|_2 \le C_2, \quad \left\|\phi^m\right\|_{H_h^1} \le C_3 \tag{9}$$

where C_1, C_2, and C_3 are positive constants independent of s, h, and T.

Proof. According to *Theorem 1*, the energy bound is given by:

$$\frac{1}{4}\|\phi\|_4^4 - \frac{1}{2}\|\phi\|_2^2 + \frac{\varepsilon^2}{2}\|\nabla_N\phi\|_2^2 \le E_N(\phi^m,\phi^{m-1}) \le E_N(\phi^0,\phi^{-1}) = E_N(\phi^0) \le C_0 \tag{10}$$

in which we applied the simplified initial value $\phi^{-1} = \phi^0$. Following the inequality for any $f \in G_N$:

$$\frac{1}{4}\| f \|_4^4 - \frac{1}{2}\| f \|_2^2 \geq \frac{1}{8}\| f \|_4^4 - \frac{1}{2}|\Omega| \tag{11}$$

since:

$$\frac{1}{8}| f |^4 - \frac{1}{2}| f |^2 + \frac{1}{2} \geq 0$$

holds at a point-wise level. Therefore, for all $m \geq 1$, it follows from the discrete energy (8) that:

$$\left\|\phi^m\right\|_4 \leq \left(8C_0 + 4|\Omega|\right)^{1/4} := C_1 \tag{12}$$

Next, according to the following fact:

$$\frac{1}{2}\left\|\phi^m\right\|_2^2 + \frac{\epsilon^2}{2}\left\|\nabla_N \phi^m\right\|_2^2 - |\Omega| \leq E_N(\phi^m) \leq C_0 \tag{13}$$

we obtain directly the estimates:

$$\left\|\phi^m\right\|_2 \leq \sqrt{2C_0 + 2|\Omega|} := C_2, \left\|\nabla_N \phi^m\right\|_2 \leq \sqrt{\frac{2C_0 + 2|\Omega|}{\epsilon^2}} := \tilde{C}_3 \tag{14}$$

Finally, applications of the Sobolev inequality and the Poincare inequality yield $\left\|\phi^m\right\|_{H_h^1} \leq C_3$.

For the term associated with the cubic non-linear part in eq. (6), the following estimate is given.

Lemma 3. Suppose that $\phi^m \in G_N$, $m = 0, 1,\ldots, M$ are defined as in *Lemma 2*. Then, we have the following estimates:

$$\left\|\Delta_N[(\phi^m)^3]\right\|_2 \leq C_4 \left\|\Delta_N^2 \phi^m\right\|_2^{2/3} \tag{15}$$

where $C_4 := 3CC_3^{7/3}$ is also independent of *s*, *h*, and *T*.

Proof. Denote ϕ_S^m is the continuous extension of the discrete grid function ϕ^m, with the interpolation formula given by (4). Due to $\Delta[(\phi_S^m)^3] \in \mathcal{P}_{3K}$, applying *Lemma 1* ($n = 3$, $d = 2$) and the Holder inequality, we have:

$$\left\|\Delta_N[(\phi^m)^3]\right\|_2 = \left\|\Delta \mathcal{I}_N[(\phi_S^m)^3]\right\|_{L^2} \leq (\sqrt{3})^2 \left\|\Delta[(\phi_S^m)^3]\right\|_{L^2} \tag{16}$$

At the same time, it follows from the standard expansion:

$$\Delta[(\phi_S^m)^3] = 3(\phi_S^m)^2 \Delta\phi_S^m + 6\phi_S^m \left|\nabla \phi_S^m\right|^2 \tag{17}$$

that:

$$\begin{aligned}\left\|\Delta[(\phi_S^m)^3]\right\|_{L^2} &\le 3C\left\|\phi_S^m\right\|_{L^6}^2\cdot\left\|\Delta\phi_S^m\right\|_{L^6}+6C\left\|\phi_S^m\right\|_{L^6}\cdot\left\|\nabla\phi_S^m\right\|_{L^6}^2\\ &\le C\left(\left\|\phi_S^m\right\|_{H^1}^2\cdot\left\|\Delta\phi_S^m\right\|_{H^1}+\left\|\phi_S^m\right\|_{H^1}\cdot\left\|\nabla\phi_S^m\right\|_{H^1}^2\right)\\ &\le C\left(C_3^2\cdot\left\|\Delta\phi_S^m\right\|_{H^1}+C_3\cdot\left\|\nabla\phi_S^m\right\|_{H^1}^2\right)\\ &\le C\left[C_3^2\cdot\left\|\nabla\phi_S^m\right\|_{L^2}^{1/3}\cdot\left\|\Delta^2\phi_S^m\right\|_{L^2}^{2/3}+C_3\cdot\left(\left\|\nabla\phi_S^m\right\|_{L^2}^{2/3}\cdot\left\|\Delta^2\phi_S^m\right\|_{L^2}^{2/3}\right)^2\right]\\ &\le CC_3^{7/3}\left\|\Delta^2\phi_S^m\right\|_{L^2}^{2/3}\end{aligned}\tag{18}$$

in which the Sobolev embedding from H^1 into L^6 and the Gagliardo-Nirenberg inequality are repeatedly applied. Hence, a combination of (16), (18) and the equality $\left\|\Delta^2\phi_S^m\right\|_{L^2}=\left\|\Delta_N^2\phi^m\right\|_2$ indicates the result (15).

We note that the $\|\cdot\|_{H_h^1}$ estimate of the numerical solutions obtained in *Lemma 2* is not sufficient to derive an maximum bound in the 2-D case for the CH equation. We need an $\|\cdot\|_{H_h^2}$ bound to obtain point-wise control of the numerical approximation.

Theorem 2 Assume an initial data $\phi^0\in H_{per}^2(\Omega)$ and $A\ge 1/16$. Then, the following bound is valid for the numerical solution given by the approximation eq. (6):

$$\|\phi\|_{\ell^\infty\left(0,T;H_h^2\right)}:=\max_{0\le m\le M}\left\|\phi_S^m\right\|_{H^2}\le\tilde{C}\tag{19}$$

where $sM = T$ and $\tilde{C}>0$ is a constant independent of h and s, but dependent of T. Moreover, the ℓ^∞ bound of the numerical solution:

$$\|\phi\|_{l^\infty(0,T;l^\infty)}\le\hat{C},\quad\forall m\ge 0\tag{20}$$

is valid.

Proof. Taking the discrete inner product of (6) with $\Delta_N^2\phi^{m+1}$ gives:

$$\begin{gathered}\left\langle\frac{3\phi^{m+1}-4\phi^m+\phi^{m-1}}{2},\Delta_N^2\phi^{m+1}\right\rangle+As^2\left\langle\Delta_N^2(\phi^{m+1}-\phi^m),\Delta_N^2\phi^{m+1}\right\rangle+\\ +\varepsilon^2 s\left\langle\Delta_N^2\phi^{m+1},\Delta_N^2\phi^{m+1}\right\rangle=\\ =s\left\langle\Delta_N(\phi^{m+1})^3,\Delta_N^2\phi^{m+1}\right\rangle-s\left\langle\Delta_N(2\phi^m-\phi^{m-1})^3,\Delta_N^2\phi^{m+1}\right\rangle+\\ Bs\left\langle\Delta_N(\phi^{m+1}-2\phi^m+\phi^{m-1}),\Delta_N^2\phi^{m+1}\right\rangle\end{gathered}\tag{21}$$

Applying the summation-by-parts with periodic boundary condition, we have:

$$\begin{aligned}
&\frac{1}{2}\left\langle 3\phi^{m+1}-4\phi^{m}+\phi^{m-1},\Delta_N^2\phi^{m+1}\right\rangle = \\
&=\frac{1}{2}\left\langle \Delta_N(3\phi^{m+1}-4\phi^{m}+\phi^{m-1}),\Delta_N\phi^{m+1}\right\rangle \geq \\
&\geq \left(\frac{3}{4}\left\|\Delta_N\phi^{m+1}\right\|_2^2-\frac{1}{4}\left\|\Delta_N\phi^{m}\right\|_2^2+\frac{1}{2}\left\|\Delta_N(\phi^{m+1}-\phi^{m})\right\|_2^2\right)- \\
&-\left(\frac{3}{4}\left\|\Delta_N\phi^{m}\right\|_2^2-\frac{1}{4}\left\|\Delta_N\phi^{m-1}\right\|_2^2+\frac{1}{2}\left\|\Delta_N(\phi^{m}-\phi^{m-1})\right\|_2^2\right)= \\
&=\mathcal{J}^{m+1}-\mathcal{J}^{m}
\end{aligned} \tag{22}$$

where $\mathcal{J}^{m+1}=\dfrac{3}{4}\left\|\Delta_N\phi^{m+1}\right\|_2^2-\dfrac{1}{4}\left\|\Delta_N\phi^{m}\right\|_2^2+\dfrac{1}{2}\left\|\Delta_N(\phi^{m+1}-\phi^{m})\right\|_2^2$.

For the stabilizing term, the following identity is valid:

$$\left\langle \Delta_N^2(\phi^{m+1}-\phi^{m}),\Delta_N^2\phi^{m+1}\right\rangle=\frac{1}{2}\left(\left\|\Delta_N^2\phi^{m+1}\right\|_2^2-\left\|\Delta_N^2\phi^{m}\right\|_2^2\right)+\frac{1}{2}\left\|\Delta_N^2(\phi^{m+1}-\phi^{m})\right\|_2^2 \tag{23}$$

Similarly, the surface diffusion term can be handled:

$$\left\langle \Delta_N^2\phi^{m+1},\Delta_N^2\phi^{m+1}\right\rangle=\left\|\Delta_N^2\phi^{m+1}\right\|_2^2 \tag{24}$$

In turn, we apply the Cauchy inequality and ε-inequality to the concave term, and get:

$$\begin{aligned}
&-\left\langle \Delta_N(2\phi^{m}-\phi^{m-1}),\Delta_N^2\phi^{m+1}\right\rangle \leq \left\|\Delta_N(2\phi^{m}-\phi^{m-1})\right\|_2\cdot\left\|\Delta_N^2\phi^{m+1}\right\|_2 \leq \\
&\leq \beta\left\|\Delta_N^2\phi^{m+1}\right\|_2^2+\frac{1}{4\beta}\left\|\Delta_N(2\phi^{m}-\phi^{m-1})\right\|_2^2 \leq \\
&\leq \beta\left\|\Delta_N^2\phi^{m+1}\right\|_2^2+\frac{2}{\beta}\left\|\Delta_N\phi^{m}\right\|_2^2+\frac{1}{2\beta}\left\|\Delta_N\phi^{m-1}\right\|_2^2 \leq \\
&\leq \beta\left\|\Delta_N^2\phi^{m+1}\right\|_2^2+2\beta\left\|\Delta_N^2\phi^{m}\right\|_2^2+\frac{\beta}{2}\left\|\Delta_N^2\phi^{m-1}\right\|_2^2+C_5(\beta)
\end{aligned} \tag{25}$$

for any $\beta \geq 0$, in which the inequality $(a+b)^2 \leq 2(a^2+b^2)$ and:

$$\left\|\Delta_N\phi^{\ell}\right\|_2^2=\left\langle \phi^{\ell},\Delta_N^2\phi^{\ell}\right\rangle \leq \frac{1}{4\beta^2}\left\|\phi^{\ell}\right\|_2^2+\beta^2\left\|\Delta_N^2\phi^{\ell}\right\|_2^2 \leq \frac{C_2^2}{4\beta^2}+\beta^2\left\|\Delta_N^2\phi^{\ell}\right\|_2^2 \tag{26}$$

For $\ell = m, m-1$ are also used.

The estimate for the last term on the RHS of eq. (21) is similar to that of the concave diffusion term. First, we will need the following weighed Sobolev inequality:

$$\left\|(-\Delta_N)^{3/2}\phi^{l}\right\|_2^2 \leq C\left\|\nabla_N\phi^{l}\right\|_2^{2/3}\left\|\Delta_N^2\phi^{l}\right\|_2^{4/3} \leq CC_3^{2/3}\left\|\Delta_N^2\phi^{l}\right\|_2^{4/3} \leq \tilde{C}_5+\frac{\beta}{B}\left\|\Delta_N^2\phi^{l}\right\|_2^2 \tag{27}$$

for any $\beta > 0$, where $\tilde{C}_5 > 0$ depends on B, β, and C_3. Then, using the summation-by-parts formula and the Cauchy inequality, we have:

$$\left\langle \Delta_N^2 \phi^{m+1}, \Delta_N (\phi^{m+1} - 2\phi^m + \phi^{m-1}) \right\rangle =$$

$$= \left\| -(-\Delta_N)^{3/2} \phi^{m+1} \right\|_2^2 + 2\left\langle (-\Delta_N)^{3/2} \phi^{m+1}, (-\Delta_N)^{3/2} \phi^m \right\rangle -$$

$$- \left\langle (-\Delta_N)^{3/2} \phi^{m+1}, (-\Delta_N)^{3/2} \phi^{m-1} \right\rangle \le$$

$$\le \frac{1}{2} \left\| (-\Delta_N)^{3/2} \phi^{m+1} \right\|_2^2 + \left\| (-\Delta_N)^{3/2} \phi^m \right\|_2^2 + \left\| \frac{1}{2} (-\Delta_N)^{3/2} \phi^{m-1} \right\|_2^2 \le$$

$$\le 3\tilde{C}_5 + \left\| \frac{\beta}{2B} \Delta_N^2 \phi^{m+1} \right\|_2^2 + \left\| \frac{\beta}{B} \Delta_N^2 \phi^m \right\|_2^2 + \left\| \frac{\beta}{2B} \Delta_N^2 \phi^{m-1} \right\|_2^2 \tag{28}$$

Next, we consider the inner product associated with the non-linear term. According to *Lemma 3*, we arrive at:

$$\left\langle \Delta_N (\phi^{m+1})^3, \Delta_N^2 \phi^{m+1} \right\rangle \le \left\| \Delta_N (\phi^{m+1})^3 \right\|_2 \cdot \left\| \Delta_N^2 \phi^{m+1} \right\|_2 \le C_4 \left\| \Delta_N^2 \phi^{m+1} \right\|_2^{5/3} \le$$

$$\le C_\varepsilon C_4^6 + \frac{\varepsilon^2}{4} \left\| \Delta_N^2 \phi^{m+1} \right\|_2^2 \le C_6 + \left\| \frac{\varepsilon^2}{4} \Delta_N^2 \phi^{m+1} \right\|_2^2 \tag{29}$$

in which $C_6 = C_\varepsilon C_4^6$ and the Young inequality ($p = 6$, $q = 6/5$) is applied in the last step. Therefore, a combination of eqs. (27)-(29) yields:

$$\mathcal{J}^{m+1} - \mathcal{J}^m + \left(\frac{As^2}{2} - \frac{3}{2}\beta s + \frac{3}{4}\varepsilon^2 s \right) \left\| \Delta_N^2 \phi^{m+1} \right\|_2^2 + \frac{As^2}{2} \left\| \Delta_N^2 (\phi^{m+1} - \phi^m) \right\|_2^2 \le$$

$$\le \left(\frac{As^2}{2} + 3\beta s \right) \left\| \Delta_N^2 \phi^m \right\|_2^2 + \beta s \left\| \Delta_N^2 \phi^{m-1} \right\|_2^2 + C_7 s \tag{30}$$

where $C_7 = C_5(\beta) + \tilde{C}_5(\beta) + C_6$ and $\mathcal{J}^m, \mathcal{J}^{m+1}$ are defined in eq. (22).

Choosing $\beta = \varepsilon^2/8$ fixes C_7 from previous inequality, we have:

$$\mathcal{J}^{m+1} - \mathcal{J}^m + \left(\frac{As^2}{2} + \frac{9}{16}\varepsilon^2 s \right) \left\| \Delta_N^2 \phi^{m+1} \right\|_2^2 + \frac{As^2}{2} \left\| \Delta_N^2 (\phi^{m+1} - \phi^m) \right\|_2^2 \le$$

$$\le \left(\frac{As^2}{2} + \frac{6}{16}\varepsilon^2 s \right) \left\| \Delta_N^2 \phi^m \right\|_2^2 + \frac{1}{8}\varepsilon^2 s \left\| \Delta_N^2 \phi^{m-1} \right\|_2^2 + C_7 s \tag{31}$$

where C_7 is a constant due to the fixed β.

Adding the term $\varepsilon^2 s\left\|\Delta_N^2\phi^m\right\|_2^2/8$ to both sides gives:

$$\mathcal{J}^{m+1}+\left(\frac{As^2}{2}+\frac{9}{16}\varepsilon^2 s\right)\left\|\Delta_N^2\phi^{m+1}\right\|_2^2+\frac{1}{8}\varepsilon^2 s\left\|\Delta_N^2\phi^m\right\|_2^2+\frac{As^2}{2}\left\|\Delta_N^2(\phi^{m+1}-\phi^m)\right\|_2^2\le$$

$$\le\mathcal{J}^m+\left(\frac{As^2}{2}+\frac{8}{16}\varepsilon^2 s\right)\left\|\Delta_N^2\phi^m\right\|_2^2+\frac{1}{8}\varepsilon^2 s\left\|\Delta_N^2\phi^{m-1}\right\|_2^2+C_7 s \tag{32}$$

Now, we define a modified energy:

$$\mathcal{H}^m:=\mathcal{J}^m+\left(\frac{As^2}{2}+\frac{8}{16}\varepsilon^2 s\right)\left\|\Delta_N^2\phi^m\right\|_2^2+\frac{1}{8}\varepsilon^2 s\left\|\Delta_N^2\phi^{m-1}\right\|_2^2 \tag{33}$$

Then, it follows that:

$$\mathcal{H}^{m+1}+\frac{1}{16}\varepsilon^2 s\left\|\Delta_N^2\phi^{m+1}\right\|_2^2+\frac{As^2}{2}\left\|\Delta_N^2(\phi^{m+1}-\phi^m)\right\|_2^2\le\mathcal{H}^m+C_7 s \tag{34}$$

which shows that:

$$\mathcal{H}^m\le\mathcal{H}^0+C_7\sum_{j=1}^{m-1}s\le\mathcal{H}^0+C_7T:=C_8 \tag{35}$$

Note that:

$$\mathcal{J}^m=\frac{3}{4}\left\|\Delta_N\phi^m\right\|_2^2-\frac{1}{4}\left\|\Delta_N\phi^{m-1}\right\|_2^2+\frac{1}{2}\left\|\Delta_N(\phi^m-\phi^{m-1})\right\|_2^2=\frac{1}{4}\left\|\Delta_N\phi^m\right\|_2^2+$$

$$+\frac{1}{4}\left\|\Delta_N(2\phi^m-\phi^{m-1})\right\|_2^2\ge\frac{1}{4}\left\|\Delta_N\phi^m\right\|_2^2.$$

Then, it follows from eqs. (31)-(35) that:

$$\left\|\Delta_N\phi^m\right\|_2^2\le 4\mathcal{J}^m\le 4\mathcal{H}^m\le 4C_8 \tag{36}$$

From *Lemma 3*, the following result is made:

$$\left\|\phi^{m+1}\right\|_2^2+\left\|\Delta_N\phi^{m+1}\right\|_2^2\le C_2^2+4C_8:=C_9$$

To conclude, we employ the elliptic regularity and have:

$$\left\|\phi_S^m\right\|_{H^2}\le C\left(\left\|\phi_S^m\right\|_{L^2}+\left\|\Delta\phi_S^m\right\|_{L^2}\right)=C\left(\left\|\phi^m\right\|_2+\left\|\Delta_N\phi^m\right\|_2\right)\le\sqrt{C_9}:=\tilde{C} \tag{37}$$

In addition, we observe the following Sobolev inequality:

$$\left\|\phi^m\right\|_\infty\le\left\|\phi_S^m\right\|_{L^\infty}\le C\left\|\phi_S^m\right\|_{H^2}\le C\tilde{C}:=C,\quad\forall m\ge 0$$

where the first estimate is based on the fact that ϕ^m is the point-wise interpolation of its continuous extension ϕ_S^m which gives the l^∞ bound of the numerical solution. This finishes the proof.

Linear iteration solver

In this section, we propose a linear iteration method to solve the eq. (6). The eq. (6) can be reformulated as a closed equation:

$$\left(\frac{3}{2}\mathcal{I}+As^2\Delta_N^2+\epsilon^2 s\Delta_N^2-Bs\Delta_N\right)\phi^{m+1}=$$

$$=s\Delta_N(\phi^{m+1})^3+\left(2\mathcal{I}-2s\Delta_N+As^2\Delta_N^2-2Bs\Delta_N\right)\phi^m+\left[(B+1)s\Delta_N-\frac{1}{2}\mathcal{I}\right]\phi^{m-1} \tag{38}$$

where $\mathcal{I}$ denotes the identity operator.

Also, define a linear operator $\mathcal{I}$ and the value f_m associated with the m^{th} and $(m-1)^{\text{th}}$ levels:

$$\mathcal{L}:=\left(\frac{3}{2}\mathcal{I}+As^2\Delta_N^2+\epsilon^2 s\Delta_N^2-Bs\Delta_N\right)$$

$$f_m:=\left(2\mathcal{I}-2s\Delta_N+As^2\Delta_N^2-2Bs\Delta_N\right)\phi^m+\left[(B+1)s\Delta_N-\frac{1}{2}\mathcal{I}\right]\phi^{m-1} \tag{39}$$

Then, eq. (38) can be simplified:

$$\mathcal{L}\phi^{m+1}=s\Delta_N(\phi^{m+1})^3+f_m \tag{40}$$

Obviously, the non-linear part in this equation is treated implicitly. To overcome the difficulty associated with the implicit treatment of the non-linear term, a linear solver is necessary, and we propose the following linear iteration algorithm:

$$\mathcal{L}\phi^{m+1,(k+1)}=s\Delta_N\left[\phi^{m+1,(k)}\right]^3+f_m \tag{41}$$

in which $\phi^{m+1,(k)}$ corresponds to the numerical solution at the k^{th} iteration.

Efficiency of iteration algorithm

We present some numerical tests to verify the efficiency of the proposed scheme compared to the CN scheme in [8] solved by the iteration algorithm (41). Different values of the diffusion coefficient ε^2 and the stability constants A, B are used.

Take the phase variable $\phi(x, y) = \sin(2\pi x)\cos(2\pi y)$ over the domain $\Omega = [0, 1]^2$ and fix $N = 128$. By setting 10^{-9} as the tolerance of iteration error, we record the average iteration time from $T = 0$ to $T = 0.5$ for eq. (6) and CN scheme in [8]. We fix $A = 1$, $B = 1$, and $\varepsilon^2 = 0.01$, 0.005, and 0.001 with different time step $s_1 = 0.01$, $s_2 = 0.005$, and $s_3 = 0.001$ and the various results are reported in tab. 1.

Table 1. The average iteration times for two schemes

	Equation (6)			CN scheme		
ε^2	s_1	s_2	s_3	s_1	s_2	s_3
0.01	6	4	2.5	5	3.6	2
0.005	10	5	2.5	12	4	2
0.001	34	12	6	130	24	2

Clearly, for small ε^2, eq. (6) costs the lest computational effort, compared to the CN scheme.

Acknowledgment

This work is supported by the Research Project of Sichuan Basic Education Research Center (No. SCJJ004) and Southwest University of Science and Technology (No. 19xn0040).

Conclusion

In this paper, we presented an energy-stable second order in time numerical scheme for the CH equation. Following the leading H^1 estimate indicated by the energy stability, we establish a uniform in time bound of the numerical solution. As a result of this H_h^2 estimate, a discrete maximum bound is also available for the numerical solution. Moreover, we also use the linear iteration algorithm in which the non-linear system can be decomposed as an iteration of purely linear solvers with more economical computational cost.

Nomenclature

x – space co-ordinate, [m]
A, B – adjustable parameters, [–]
∇ – divergence operator, [–]
Δ_N – discrete Laplacian operator, [–]
Ω – domain, [m^3]
$f_{l,m}$ – Fourier coefficient, [–]
E – energy functional, [–]
h – spatial step size, [m]

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Paper submitted: June 15, 2021
Paper revised: July 12, 2021
Paper accepted: July 21, 2021