

Research Article

A Simple Benchmark Problem for the Numerical Methods of the Cahn–Hilliard Equation

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We present a very simple benchmark problem for the numerical methods of the Cahn–Hilliard (CH) equation. For the benchmark problem, we consider a cosine function as the initial condition. The periodic sinusoidal profile satisfies both the homogeneous and periodic boundary conditions. The strength of the proposed problem is that it is simpler than the previous works. For the benchmark numerical solution of the CH equation, we use a fourth-order Runge–Kutta method (RK4) for the temporal integration and a centered finite difference scheme for the spatial differential operator. Using the proposed benchmark problem solution, we perform the convergence tests for an unconditionally gradient stable scheme via linear convex splitting proposed by Eyre and the Crank–Nicolson scheme. We obtain the expected convergence rates in time for the numerical schemes for the one-, two-, and three-dimensional CH equations.

1. Introduction

We present a very simple benchmark problem for the numerical methods of the following Cahn–Hilliard (CH) equation [1–3]:

$$\frac{\partial \phi(x, t)}{\partial t} = \Delta [F'(\phi(x, t)) - \varepsilon^2 \Delta \phi(x, t)], \quad (x, t) \in \Omega \times (0, T], \quad (1)$$

where $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) is a bounded domain, $\phi(x, t)$ is a compositional field, $F(\phi) = 0.25(\phi^2 - 1)^2$, and ε is a positive constant. The CH equation was proposed for a model of the spinodal decomposition in a binary mixture and has been used to model many scientific phenomena such as topology optimization [4], phase separation [5–7], image processing [8], two-phase fluid flows [9, 10], crystal model [11], tumor growth [12, 13], and microstructure formations (see [14] for the basic principles and practical applications and [3] for the physical, mathematical, and numerical derivations of the CH equation).

There have been many research papers regarding the accurate numerical methods for the CH equation [15–18] (see the references therein for more details). In particular, a comparison study among various numerical methods for the CH equation was conducted on the perspective of stability and efficiency [19]. A test set developed to verify models, algorithms, or the accuracy of numerical methods is called “benchmark problem” [20]. However, there are only few benchmark problems for validating the accuracy of the proposed numerical methods. Recently, the authors in [21] proposed a benchmark problem for the two- and three-dimensional CH equations. The benchmark problems were the shrinking annulus and spherical shell in the two- and three-dimensional cases, respectively. They used the explicit Euler scheme with a very fine time step size, $\Delta t < 10^{-5}$. The authors in [22] presented four benchmark problems for the Allen–Cahn (AC) and CH equations. The benchmark is the time T at which the value at a point in the domain changes from negative to positive. The authors in [20] presented two benchmark problems for phase-field models of solute diffusion and phase separation. Recently, a verification method

for the convergence rates of the numerical solutions for well-known parabolic partial differential equations was proposed in [23].

Typically, benchmark testing is essential for comparing the performance of a method. However, many researchers conduct self-tests using their own methods in most cases. There is a problem such that an error may occur relatively compared to the actual solution because an approximated solution converges to a numerical solution via an employed numerical method although convergence of a solution through numerical analysis is guaranteed. Moreover, most of these testing schemes are often implicit methods, which have relatively low accuracy compared to the results of long time simulation of explicit methods with a small time step. Therefore, the main purpose of this paper is to present a very simple benchmark problem for the numerical methods of the CH equation, which does not employ the self-test but a classical explicit method for the temporal discretization. The strength of the proposed problem is that it is simpler than the previous works [20–22]. Furthermore, the benchmark problem can be applied to both Neumann and periodic boundary conditions.

The contents of this paper are summarized as follows. In Section 2, a numerical solution is presented. In Section 3, numerical results are shown. Conclusions are made in Section 4.

2. Numerical Solution

We consider two discretization schemes to the CH equation for benchmark problem; one is the linearly stabilized splitting scheme (LSS) proposed by Eyre [24] which is first-order accurate in time and the other is the Crank–Nicolson (CN) scheme [25] which is second-order in time. In order to perform a benchmark test for these two methods, we first need to obtain a benchmark numerical solution. To obtain the benchmark solution, we consider the one-dimensional CH equation:

$$\begin{aligned} \phi_t(x, t) &= \left[F'(\phi(x, t)) - \varepsilon^2 \phi_{xx}(x, t) \right]_{xx}, \\ (x, t) &\in (0, 1) \times (0, T], \end{aligned} \quad (2)$$

with the homogeneous Neumann boundary condition $\phi_x(0, t) = \phi_x(1, t) = \phi_{xxx}(0, t) = \phi_{xxx}(1, t) = 0$. Let $h = 1/N_x$ be the uniform spatial step size, $x_i = (i - 0.5)h$ for $1 \leq i \leq N_x$, and $t_n = n\Delta t_{\text{ref}}$, where $\Delta t_{\text{ref}} = T/N_t$ is the reference time step and T is the final time. We define ϕ_i^n as an approximation of $\phi(x_i, t_n)$. Now, we discretize equation (2) in time using a fourth-order Runge–Kutta method (RK4) [26] as follows:

$$\begin{aligned} \alpha_i^n &= \Delta t_{\text{ref}} \Delta_h \left[F'(\phi_i^n) - \varepsilon^2 \Delta_h \phi_i^n \right], \\ \beta_i^n &= \Delta t_{\text{ref}} \Delta_h \left[F'(\phi_i^n + 0.5\alpha_i^n) - \varepsilon^2 \Delta_h (\phi_i^n + 0.5\alpha_i^n) \right], \\ \gamma_i^n &= \Delta t_{\text{ref}} \Delta_h \left[F'(\phi_i^n + 0.5\beta_i^n) - \varepsilon^2 \Delta_h (\phi_i^n + 0.5\beta_i^n) \right], \\ \delta_i^n &= \Delta t_{\text{ref}} \Delta_h \left[F'(\phi_i^n + \gamma_i^n) - \varepsilon^2 \Delta_h (\phi_i^n + \gamma_i^n) \right], \\ \phi_i^{n+1} &= \phi_i^n + \frac{1}{6} (\alpha_i^n + 2\beta_i^n + 2\gamma_i^n + \delta_i^n), \quad \text{for } i = 1, 2, \dots, N_x, \end{aligned} \quad (3)$$

where $\Delta_h \psi_i = (\psi_{i-1} - 2\psi_i + \psi_{i+1})/h^2$ is the standard discrete Laplacian with $\psi_0 = \psi_1$ and $\psi_{N_x+1} = \psi_{N_x}$.

3. Numerical Results

3.1. Convergence and Stability Tests. First, we conduct a traditional convergence test. As a concrete example, an initial condition is given by

$$\phi(x, 0) = 0.1 \cos(2\pi x) \text{ on } x \in \Omega = (0, 1). \quad (4)$$

Note that equation (4) can be used in testing numerical schemes with both the Neumann and periodic boundary conditions. We employ $\varepsilon = 16h/(2\sqrt{2} \tanh^{-1}(0.9)) \approx 0.03$, which is the approximate transition layer width [27]. Table 1 shows the rate of convergence. We measure the accuracy of time at the final time T using $\|e^{\Delta t, 0.5\Delta t}\|_2$ which is defined as follows:

$$\|e^{\Delta t, \Delta t/2}\|_2 = \sqrt{\frac{1}{N_x} \sum_{i=1}^{N_x} (e_i^{\Delta t, \Delta t/2})^2}, \quad (5)$$

where $e_i^{\Delta t, \Delta t/2}$ is an error between the computed solutions using large and small time steps, respectively. More precisely, it is

$$e_i^{\Delta t, \Delta t/2} = \left| \phi_i^{\Delta t} - \phi_i^{\Delta t/2} \right|. \quad (6)$$

In this test, we adopt the space step size as $h = 1/10$ and the final time as $T = 10h^4$. We can confirm that RK4 is of fourth-order in time indeed according to Table 1.

For the next test, we investigate the maximum time step sizes Δt_c with respect to the spatial step size h . Here, we fix $N_t = 10^5$ and other parameters and the initial condition are the same as those described above. Table 2 lists the largest time step sizes satisfying that the numerical solution does not blow up.

Figure 1 depicts the practically stable region and maximum time step size Δt_c as described in Table 2. The explicit scheme is theoretically $\Delta t \approx O(h^4)$.

TABLE 1: Rate of convergence of RK4.

| $(\Delta t, \Delta t/2)$ | $(h^4, h^4/2)$ | Rate | $(h^4/2, th^4/4)$ | Rate | $(h^4/4, h^4/8)$ |
|----------------------------------|----------------|-------|-------------------|-------|------------------|
| $\ e^{\Delta t, \Delta t/2}\ _2$ | 4.378e-11 | 4.030 | 2.681e-12 | 4.097 | 1.567e-13 |

TABLE 2: Practical maximum time step size Δt_c with respect to h .

| h | 1/16 | 1/32 | 1/64 | 1/128 |
|--------------|----------|----------|----------|----------|
| Δt_c | 4.686e-5 | 1.152e-5 | 2.810e-6 | 7.085e-7 |

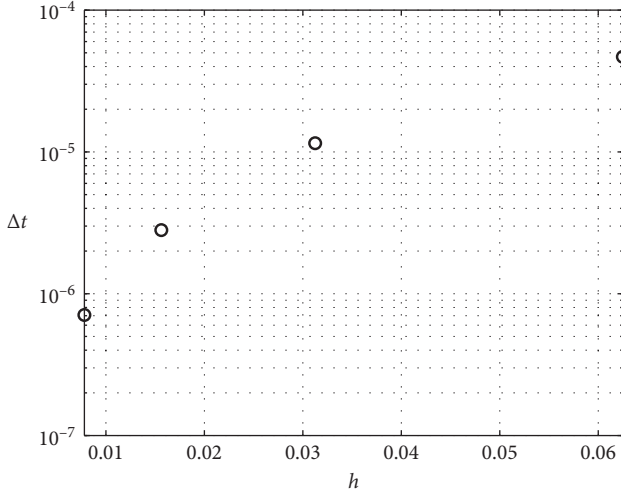
FIGURE 1: Practical maximum time step size Δt_c with respect to h .

Figure 2 represents the CPU times (seconds) with respect to the number of spatial step N_x , performed on Intel Core i5-6400 CPU at 2.70 GHz with 4 GB RAM. When we vary N_x as 16, 32, 64, and 128 with fixed parameters, $\Delta t = (1/128)^4$ and $N_t = 10^7$, the CPU times are 88.812, 175.468, 354.14, and 708.718. That is, when N_x is doubled, the CPU time is approximately doubled.

3.2. Benchmark Problem. Let us consider the benchmark problem for the CH equation. We adopt equation (4) as an initial condition. For the reference numerical solution of the benchmark problem, we use $h = 1/128$, $\Delta t_{\text{ref}} = h^4$, and $N_t = 10^7$. Therefore, the final time is $T = N_t \Delta t_{\text{ref}} = 10^7 h^4$. For the model parameter, we use $\varepsilon = 24h/(2\sqrt{2} \tanh^{-1}(0.9)) \approx 0.045$. Figure 3 shows the initial condition and the reference numerical solution at $t = 10^7 h^4$.

3.2.1. One-Dimensional Space. Let us define an error $e(x, T)$ as the difference between $\phi_{\Delta t}$ and $\phi_{\Delta t_{\text{ref}}}$ at the final time T , i.e., $e(x, T) = |\phi_{\Delta t}(x, T) - \phi_{\Delta t_{\text{ref}}}(x, T)|$, where $\phi_{\Delta t}$ and $\phi_{\Delta t_{\text{ref}}}$ are the numerical solution with a time step Δt and the reference numerical solution with a time step Δt_{ref} , respectively. The one-dimensional LSS and CN schemes to be benchmarked are as follows:

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \Delta_h \left[(\phi_i^n)^3 - 3\phi_i^n + 2\phi_i^{n+1} - \varepsilon^2 \Delta_h \phi_i^{n+1} \right], \quad (7)$$

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{1}{2} \Delta_h \left[(\phi_i^n)^3 - \phi_i^n - \varepsilon^2 \Delta_h \phi_i^n + (\phi_i^{n+1})^3 - \phi_i^{n+1} - \varepsilon^2 \Delta_h \phi_i^{n+1} \right], \quad (8)$$

where Δt is a time step. We solve equations (7) and (8) using a multigrid method [25, 28]. Note that we use the Gauss-Seidel iterative method in multigrid process combined with Newton's approximation to compute the nonlinear term in equation (8). Figures 4(a) and 4(b) show the errors for the LSS and CN scheme, respectively.

Now, we define the discrete l_2 -norm and the discrete maximum norm as

$$\|e\|_2 = \sqrt{\frac{1}{N_x} \sum_{i=1}^{N_x} e_i^2}, \quad (9)$$

$$\|e\|_\infty = \max_{1 \leq i \leq N_x} e_i,$$

respectively. Tables 3 and 4 list the numerical errors and convergence rates of the LSS and those of the CN scheme at $t = 10^7 h^4$, respectively. We confirm that both the schemes achieve the expected convergence rates (the first-order for the LSS and the second-order for the CN scheme).

3.2.2. Two-Dimensional Space. Next, we consider the two-dimensional version of equations (7) and (8) to the CH equation on $\Omega = (0, 1) \times (0, 1)$. Straightforward extensions of the LSS and CN schemes are as follows:

$$\frac{\phi_{ij}^{n+1} - \phi_{ij}^n}{\Delta t} = \Delta_h \left[(\phi_{ij}^n)^3 - 3\phi_{ij}^n + 2\phi_{ij}^{n+1} - \varepsilon^2 \Delta_h \phi_{ij}^{n+1} \right], \quad (10)$$

$$\frac{\phi_{ij}^{n+1} - \phi_{ij}^n}{\Delta t} = \frac{1}{2} \Delta_h \left[(\phi_{ij}^n)^3 - \phi_{ij}^n - \varepsilon^2 \Delta_h \phi_{ij}^n + (\phi_{ij}^{n+1})^3 - \phi_{ij}^{n+1} - \varepsilon^2 \Delta_h \phi_{ij}^{n+1} \right], \quad (11)$$

where $\Delta_h \psi_{ij} = (\psi_{i-1,j} + \psi_{i+1,j} + \psi_{i,j-1} + \psi_{i,j+1} - 4\psi_{ij})/h^2$ and $h = 1/N_x = 1/N_y = 1/128$. We denote $\phi(x, y, t_n) = \phi((i-0.5)h, (j-0.5)h, n\Delta t)$ by ϕ_{ij}^n for $i = 1, \dots, N_x$ and $j = 1, \dots, N_y$. An initial condition is given by a simple extension of equation (4):

$$\phi(x, y, 0) = 0.1 \cos(2\pi x) \text{ on } \Omega. \quad (12)$$

We can minimize the influence of domain in this way. Therefore, the two-dimensional reference numerical solution is extended from that of the one-dimensional as follows:

$$\phi_{ij} = \phi_i, \quad \text{for } 1 \leq i \leq N_x, 1 \leq j \leq N_y. \quad (13)$$

Figures 5(a) and 5(b) show the initial condition and the reference solution at $t = 10^7 h^4$, respectively.

We define the discrete l_2 -norm and the discrete maximum norm as

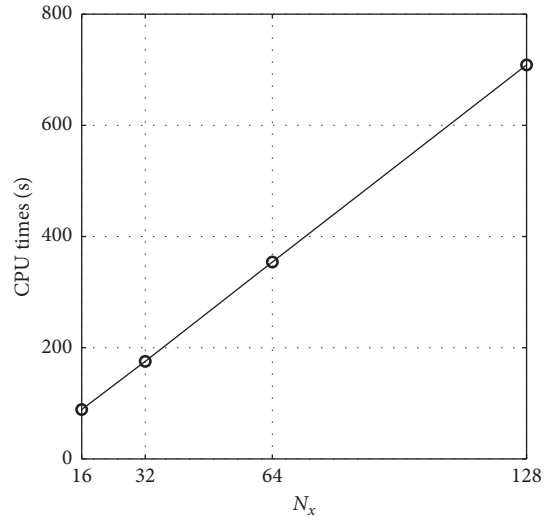
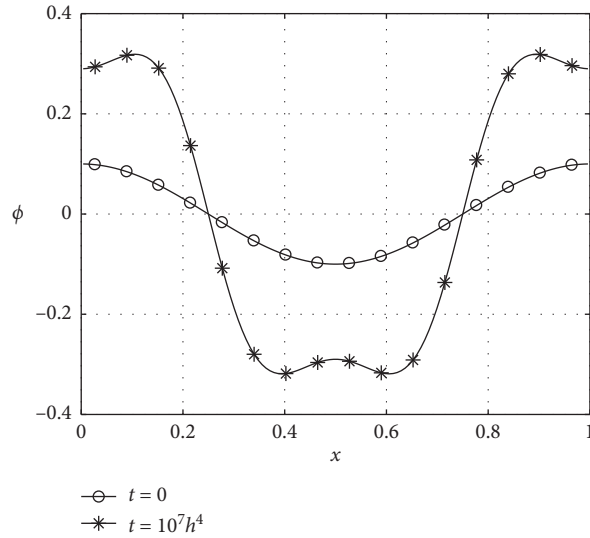


FIGURE 2: CPU times versus spatial step.

FIGURE 3: Initial condition and the reference numerical solution at $t = 10^7 h^4$.

$$\|e\|_2 = \sqrt{\frac{1}{N_x N_y} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} e_{ij}^2}, \quad (14)$$

$$\|e\|_\infty = \max_{\substack{1 \leq i \leq N_x \\ 1 \leq j \leq N_y}} e_{ij},$$

respectively. Tables 5 and 6 list the errors and convergence rates of the numerical results at $t = 10^7 h^4$. From the results,

we observe that both the schemes achieve the expected convergence rates (the first-order for LSS (10) and the second-order for CN scheme (11)).

3.2.3. Three-Dimensional Space. Finally, the two numerical schemes are extended to the three-dimensional CH equation as follows:

$$\frac{\phi_{ijk}^{n+1} - \phi_{ijk}^n}{\Delta t} = \Delta_h \left[(\phi_{ijk}^n)^3 - 3\phi_{ijk}^n + 2\phi_{ijk}^{n+1} - \varepsilon^2 \Delta_h \phi_{ijk}^{n+1} \right], \quad (15)$$

$$\frac{\phi_{ijk}^{n+1} - \phi_{ijk}^n}{\Delta t} = \frac{1}{2} \Delta_h \left[\left[(\phi_{ijk}^n)^3 - \phi_{ijk}^n - \varepsilon^2 \Delta_h \phi_{ijk}^n + (\phi_{ijk}^{n+1})^3 - \phi_{ijk}^{n+1} - \varepsilon^2 \Delta_h \phi_{ijk}^{n+1} \right] \right], \quad (16)$$

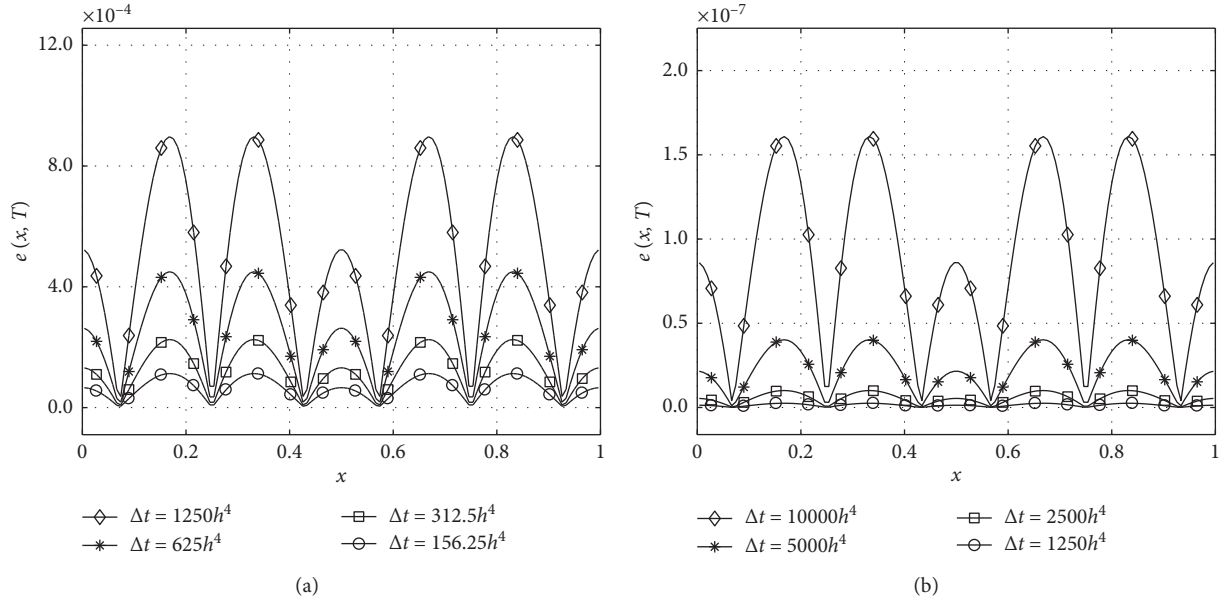


FIGURE 4: Errors between the reference solution and the solutions evaluated using (a) the LSS and (b) the CN scheme at $t = 10^7 h^4$.

TABLE 3: Errors and convergence rates for the numerical results of the LSS at the final time $T = 10^7 h^4$. Here, $h = 1/128$ is used.

| Δt | $1250h^4$ | Rate | $625h^4$ | Rate | $312.5h^4$ | Rate | $156.25h^4$ |
|----------------|------------|-------|------------|-------|------------|-------|-------------|
| $\ e\ _2$ | $5.687e-4$ | 0.995 | $2.854e-4$ | 0.997 | $1.430e-4$ | 0.999 | $7.150e-5$ |
| $\ e\ _\infty$ | $8.970e-4$ | 0.995 | $4.500e-4$ | 0.998 | $2.254e-4$ | 0.999 | $1.128e-4$ |

TABLE 4: Errors and convergence rates for the numerical results of the CN scheme at the final time $T = 10^7 h^4$. Here, $h = 1/128$ is used.

| Δt | $10000h^4$ | Rate | $5000h^4$ | Rate | $2500h^4$ | Rate | $1250h^4$ |
|----------------|------------|-------|------------|-------|------------|-------|------------|
| $\ e\ _2$ | $1.014e-7$ | 2.000 | $2.540e-8$ | 2.000 | $6.300e-9$ | 2.001 | $1.600e-9$ |
| $\ e\ _\infty$ | $1.608e-7$ | 2.000 | $4.020e-8$ | 2.000 | $1.010e-8$ | 2.000 | $2.500e-9$ |

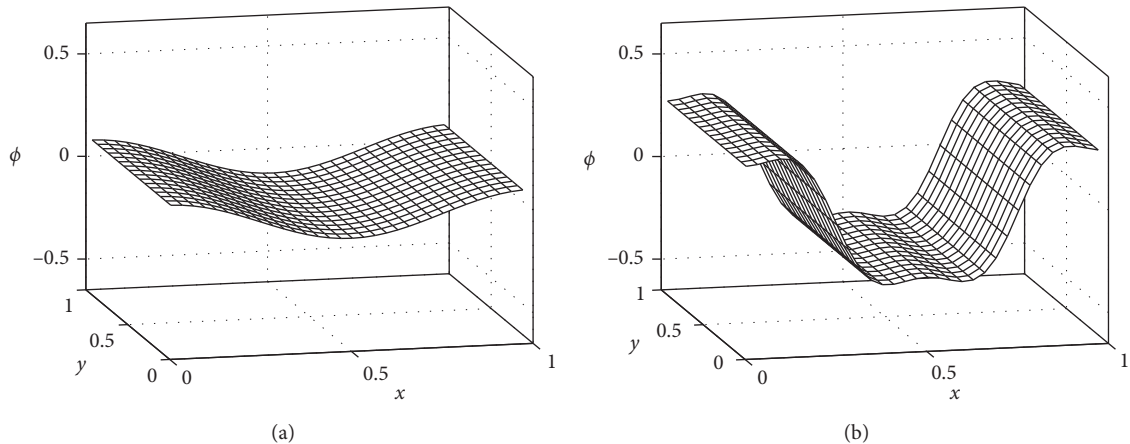


FIGURE 5: (a, b) The initial condition and the reference solution at $t = 10^7 h^4$, respectively.

where $\Delta_h \phi_{ijk} = (\phi_{i-1,jk} + \phi_{i+1,jk} + \phi_{i,j-1,k} + \phi_{i,j+1,k} + \phi_{i,j,k-1} + \phi_{i,j,k+1} - 6\phi_{ijk})/h^2$. Here, $h = 1/N_x = 1/N_y = 1/N_z = 1/128$. An initial condition is given by

$$\phi(x, y, z, 0) = 0.1 \cos(2\pi x) \text{ on } \Omega = (0, 1)^3. \quad (17)$$

We extend the one-dimensional reference solution to the three-dimensional reference numerical solution:

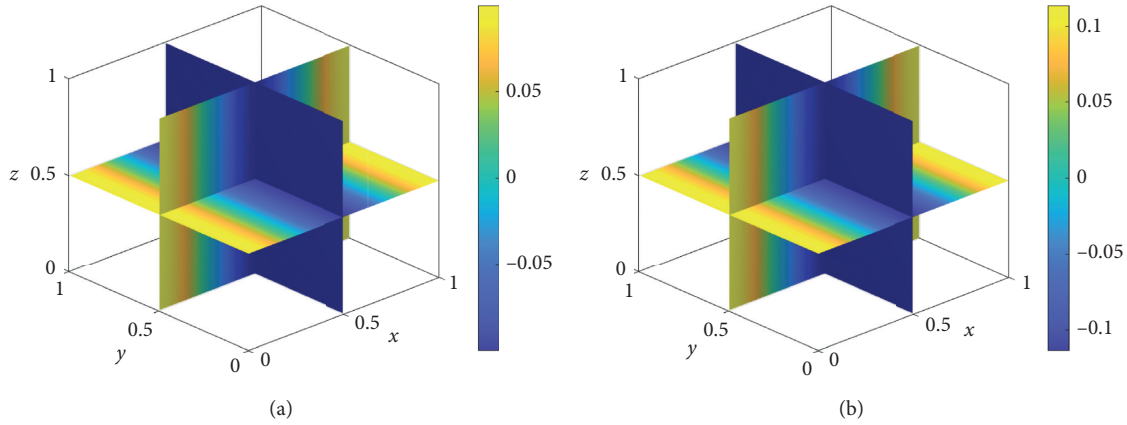
$$\phi_{ijk} = \phi_i, \quad \text{for } 1 \leq i \leq N_x, 1 \leq j \leq N_y, 1 \leq k \leq N_z. \quad (18)$$

TABLE 5: Errors and convergence rates for the numerical results of the LSS at the final time $T = 10^7 h^4$. Here, $h = 1/128$ is used.

| Δt | $2500h^4$ | Rate | $1250h^4$ | Rate | $625h^4$ | Rate | $312.5h^4$ |
|----------------|-----------|-------|-----------|-------|----------|-------|------------|
| $\ e\ _2$ | 0.0011 | 0.990 | 0.0006 | 0.995 | 0.0003 | 0.997 | 0.0001 |
| $\ e\ _\infty$ | 0.0018 | 0.990 | 0.0009 | 0.995 | 0.0005 | 0.998 | 0.0002 |

TABLE 6: Errors and convergence rates for the numerical results of the CN scheme at the final time $T = 10^7 h^4$. Here, $h = 1/128$ is used.

| Δt | $10000h^4$ | Rate | $5000h^4$ | Rate | $2500h^4$ | Rate | $1250h^4$ |
|----------------|------------|-------|------------|-------|------------|-------|------------|
| $\ e\ _2$ | $1.014e-7$ | 2.000 | $2.540e-8$ | 2.000 | $6.300e-9$ | 1.999 | $1.600e-9$ |
| $\ e\ _\infty$ | $1.608e-7$ | 2.000 | $4.020e-8$ | 1.999 | $1.010e-8$ | 1.997 | $2.500e-9$ |

FIGURE 6: (a, b) The initial condition and the reference solution at $t = 10^6 h^4$, respectively.TABLE 7: Errors and convergence rates for the numerical results of the LSS at the final time $T = 10^6 h^4$. Here, $h = 1/128$ is used.

| Δt | $10000h^4$ | Rate | $5000h^4$ | Rate | $2500h^4$ | Rate | $1250h^4$ |
|----------------|------------|-------|------------|-------|------------|-------|------------|
| $\ e\ _2$ | $4.287e-5$ | 0.994 | $2.153e-5$ | 0.997 | $1.079e-5$ | 0.998 | $5.400e-6$ |
| $\ e\ _\infty$ | $5.522e-5$ | 0.990 | $2.782e-5$ | 0.995 | $1.397e-5$ | 0.997 | $7.000e-6$ |

TABLE 8: Errors and convergence rates for the numerical results of the CN scheme at the final time $T = 10^6 h^4$. Here, $h = 1/128$ is used.

| Δt | $10000h^4$ | Rate | $5000h^4$ | Rate | $2500h^4$ | Rate | $1250h^4$ |
|----------------|------------|-------|-------------|-------|-------------|-------|-------------|
| $\ e\ _2$ | $1.911e-9$ | 2.000 | $4.780e-10$ | 2.000 | $1.190e-10$ | 1.999 | $3.000e-11$ |
| $\ e\ _\infty$ | $2.860e-9$ | 2.000 | $7.150e-10$ | 1.998 | $1.790e-10$ | 1.955 | $4.600e-11$ |

Note that the final time T is set to $10^6 h^4$ for ease of computation in the three-dimensional space. Figures 6(a) and 6(b) show the initial condition and the reference solution at $t = 10^6 h^4$, respectively.

The discrete l_2 -norm and the discrete maximum norm are simply extended as follows:

$$\|e\|_2 = \sqrt{\frac{1}{N_x N_y N_z} \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} e_{ijk}^2}, \quad (19)$$

$$\|e\|_\infty = \max_{1 \leq i \leq N_x, 1 \leq j \leq N_y, 1 \leq k \leq N_z} e_{ijk},$$

respectively. Tables 7 and 8 list errors and convergence rates for the numerical results at $t = 10^6 h^4$. Tables 7 and 8 show

that equations (15) and (16) are of first-order and of second-order in time, respectively.

4. Conclusions

In this work, we proposed a very simple benchmark problem, which is a cosine function as the initial condition for the numerical methods of the CH equations. For the numerical solution, we used RK4 for the temporal integration. Using the proposed benchmark problem solution, we performed the convergence tests for LSS and CN schemes and obtained the expected first-order and second-order convergence rates in the one-, two-, and three-dimensional CH equations, respectively. The proposed approach is less biased and provides more rational results compared to conventional self-convergence tests. In future work, we will

design simple benchmark problems for other nonlinear partial differential equations such as the nonlocal CH, AC, and nonlocal AC equations.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare no conflicts of interest.

Acknowledgments

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