Thesis for the Degree of Master

A fourth-order compact finite difference method for the Cahn-Hilliard equation
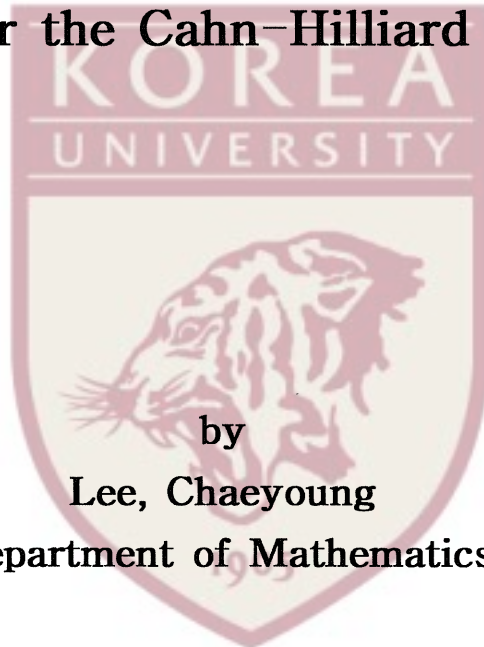
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碩 士 學 位 論 文

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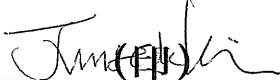
이 論文을 理學碩士學位 論文으로 提出함.

2014 年 6 月

高麗大學校 大學院
數學科
李 宋 瑛

李宋瑛의 理學碩士學位 論文
審査를 完了함.

2014 年 6 月 日

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Abstract

A fourth-order accurate and practically stable compact finite difference method is proposed for the Cahn–Hilliard equation.

We present a compact finite difference stencil of the Laplacian operator in two-dimension. It is applied to the Poisson and heat equations and perform numerical experiments to verify their fourth-order accuracy. And, we present the compact scheme for the linearly stabilized splitting scheme for the Cahn–Hilliard equation. It is fourth-order accurate and practically stable. We solve the resulting system of discrete equations by a multigrid method. There are a variety of numerical experiments to show the fourth-order convergence, non-increase of total energy, mass conservation, linear stability analysis, robustness of the scheme, and evolution up to the steady state. Also, we demonstrate that the proposed scheme is more robust and efficient than the non-compact fourth-order scheme.

This thesis includes the contents in the following publication: "A fourth-order spatial accurate and practically stable compact scheme for the Cahn–Hilliard equation." Physica A: Statistical Mechanics and its Applications 409 (2014) 17–28.

Chapter 1

Introduction

The Cahn–Hilliard equation was originally introduced as a phenomenological model of phase separation in a binary alloy [1, 2] and has been widely applied in many areas such as image processing [3, 4], microstructure [5], multi-phase fluid flows [6], planet formation [7], and tumor growth [8, 9]. The Cahn–Hilliard equation is

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \nabla \cdot [M(\phi(\mathbf{x}, t))\nabla \mu(\phi(\mathbf{x}, t))], \quad \mathbf{x} \in \Omega, \quad t > 0, \qquad (1.1)$$

$$\mu(\phi(\mathbf{x}, t)) = F'(\phi(\mathbf{x}, t)) - \epsilon^2 \Delta \phi(\mathbf{x}, t), \qquad (1.2)$$

where Ω is a bounded domain that satisfies periodic boundary conditions for ϕ and μ. The quantity $\phi(\mathbf{x}, t)$ is a phase-field order parameter, which is defined as the difference of mass concentrations of the components in a binary mixture. μ is a chemical potential and M is a mobility. The free energy density

$$F(\phi) = \frac{1}{4}(\phi^2 - 1)^2$$

has a double-well potential that has two local minima at the minimum and maximum of the concentration as shown in Figure 1.1. ϵ is a positive constant related to the interfacial thickness. The total free energy functional of the Cahn–Hilliard equation
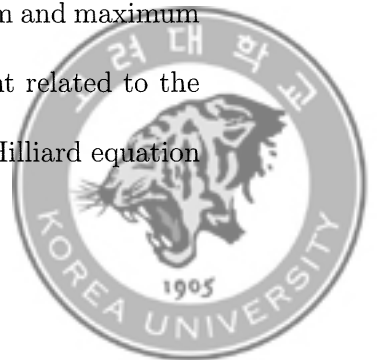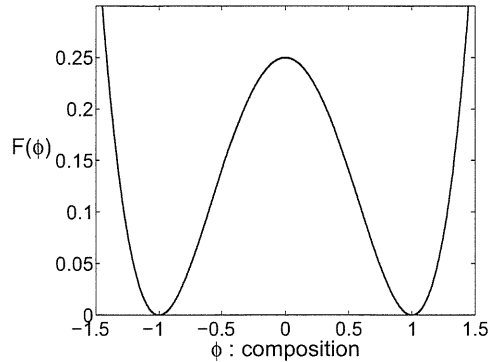
FIGURE 1.1. Free energy density $F(\phi)$

is defined as

$$\mathcal{E}(\phi) = \int_\Omega \left(F(\phi) + \frac{\epsilon^2}{2} |\nabla \phi|^2 \right) d\mathbf{x}.$$

We differentiate the energy $\mathcal{E}(t)$ with respect to t and the total mass $\int_\Omega \phi d\mathbf{x}$ using the boundary condition,

$$\frac{d}{dt}\mathcal{E}(t) \leq 0 \quad \text{and} \quad \frac{d}{dt}\int_\Omega \phi d\mathbf{x} = 0.$$

Therefore, the total energy is non-increasing in time t and the total mass is conserved.

The Cahn–Hilliard equation has fourth-order spatial derivatives and a Laplacian acting on the nonlinear term $F'(\phi)$. In general, explicit time discretizations require small time step sizes for stability. To overcome constraints of the time step sizes, several implicit time discretizations have been proposed [10, 11, 12, 13, 14, 15, 16]. However, most of these numerical solutions have the second-order accuracy in spatial discretizations. Note that the spectral [17, 18, 19] and finite element [20] methods for

$$- 2 -$$

the Cahn–Hilliard equation can be approximated to arbitrary accuracy. However, there are advantages and disadvantages to each numerical method.

In recent years, high-order compact difference methods have been developed for simulating computational fluid dynamics [22], acoustics [23], electromagnetic [24, 25], and option pricing in stochastic volatility models [26]. Moreover, there are various studies about fourth-order compact schemes for the Poisson [27, 28, 29], heat [30], Navier–Stokes [31, 32, 33], biharmonic [34, 35], reaction-diffusion [36], and convection-diffusion [37, 38] equations. Also, sixth-order compact schemes for the Poisson [29, 39], Helmholtz [24], and convection-diffusion equations [22] have been developed. Up to now, there are many works on the second-order finite difference method but few works on the high-order difference method for the Cahn–Hilliard equation. Li *et al.* [40] established a three-level linearized compact difference scheme for the Cahn–Hilliard equation. In this thesis, we propose the compact scheme by combining a compact nine-point formula and linearly stabilized splitting scheme [41].

This thesis is organized as follows. In Chapter 2, we derive a fourth-order compact finite difference scheme. We consider the compact scheme for the Poisson and heat equations. In Chapter 3, the fourth-order accurate and practically stable compact scheme is presented for the Cahn–Hilliard equation. And, we describe the multigrid algorithm for the resulting system. In Chapter 4, there are various numerical experiments to demonstrate. Finally, conclusions are drawn in Chapter 5.
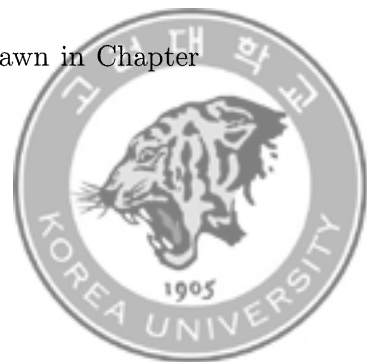
Chapter 2

Fourth-order compact finite difference scheme

2.1. Numerical discretization

We consider discretizations in two-dimensional domain $\Omega = (a, b) \times (c, d)$. Let N_x and N_y be positive even integers, $h = (b - a)/N_x = (d - c)/N_y$ be the uniform mesh size. We denote a discrete computational domain by $\Omega_h = \{(x_i, y_j) : x_i = a + (i - 0.5)h, \ y_j = c + (j - 0.5)h, \ 1 \leq i \leq N_x, \ 1 \leq j \leq N_y\}$, which is the set of cell-centers. Let ϕ_{ij}^n be the approximation of $\phi(x_i, y_j, n\Delta t)$, where $\Delta t = T/N_t$ is the time step, T is the final time, and N_t is the total number of time steps. We use periodic boundary conditions for ϕ and μ as follows:

$$\phi_{i0} = \phi_{i,Nx}, \ \phi_{i,Nx+1} = \phi_{i1}, \ \phi_{0j} = \phi_{Ny,j}, \ \phi_{Ny+1,j} = \phi_{1j}.$$

The discrete differentiation operators are

$$
\begin{aligned}
D_x \phi_{i+\frac{1}{2},j} &= \frac{1}{12}\frac{\phi_{i+1,j+1} - \phi_{i,j+1}}{h} + \frac{5}{6}\frac{\phi_{i+1,j} - \phi_{ij}}{h} + \frac{1}{12}\frac{\phi_{i+1,j-1} - \phi_{i,j-1}}{h}, \\
D_y \phi_{i,j+\frac{1}{2}} &= \frac{1}{12}\frac{\phi_{i+1,j+1} - \phi_{i+1,j}}{h} + \frac{5}{6}\frac{\phi_{i,j+1} - \phi_{ij}}{h} + \frac{1}{12}\frac{\phi_{i-1,j+1} - \phi_{i-1,j}}{h},
\end{aligned}
$$

and we use the notation $\nabla_c \phi_{ij} = \left(D_x \phi_{i+\frac{1}{2},j}, D_y \phi_{i,j+\frac{1}{2}} \right)$ to represent the discrete gradient of ϕ (see Figure 2.1). The discrete divergence operator is defined at cell-

(a) $D_x\phi_{i+\frac{1}{2},j}$ (b) $D_y\phi_{i,j+\frac{1}{2}}$

FIGURE 2.1. Discrete gradient of ϕ at a point ($\blacklozenge$) is a combination of six circles ($\bullet$).

center point as

$$\nabla_d \cdot (u,v)_{ij} = \frac{u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}}{h} + \frac{v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}}{h}.$$

We then define the discrete l_2-inner products as

$$(\phi,\psi)_h := h^2 \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \phi_{ij}\psi_{ij},$$

$$(\nabla_c\phi, \nabla_c\psi)_e := h^2 \sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \left(D_x\phi_{i+\frac{1}{2},j} D_x\psi_{i+\frac{1}{2},j} + D_y\phi_{i,j+\frac{1}{2}} D_y\psi_{i,j+\frac{1}{2}} \right),$$

and the discrete norms as $\|\phi\|^2 = (\phi,\phi)_h$ and $\|\nabla\phi\|_e^2 = (\nabla_c\phi, \nabla_c\phi)_e$.

The compact nine-point Laplacian operator Δ_c [42] is defined as

$$\begin{aligned}
\Delta_c\phi_{ij} &= \nabla_d \cdot \nabla_c\phi_{ij} \\
&= \frac{1}{6h^2} (\phi_{i-1,j+1} + 4\phi_{i,j+1} + \phi_{i+1,j+1} + 4\phi_{i-1,j} \\
&\quad -20\phi_{ij} + 4\phi_{i+1,j} + \phi_{i-1,j-1} + 4\phi_{i,j-1} + \phi_{i+1,j-1}),
\end{aligned}$$

(2.1)

and its stencil for the discrete Laplacian operator is illustrated in Figure 2.2(c).

FIGURE 2.2. Two-dimensional computational grids indicate (a) the five-point stencil, (b) the standard nine-point stencil, and (c) the compact nine-point stencil for the Laplacian operator at (x_i, y_j).

By using the Taylor series in two variables, we can obtain

$$\phi(x + \Delta x, y + \Delta y) = \sum_{k=0}^{5} \frac{1}{k!} \left(\Delta x \frac{\partial}{\partial x} + \Delta y \frac{\partial}{\partial y} \right)^k \phi(x, y)$$
$$+ O((\Delta x)^6 + (\Delta y)^6).$$

By replacing Δx and Δy with different values $\pm h$, we get

$$\phi(x + h, y) + \phi(x - h, y) + \phi(x, y - h) + \phi(x, y + h)$$

$$= 4\phi + h^2 \phi_{xx} + h^2 \phi_{yy} + \frac{h^4}{12} \phi_{xxxx} + \frac{h^4}{12} \phi_{yyyy} + O(h^6), \qquad (2.2)$$

$$\phi(x - h, y - h) + \phi(x - h, y + h) + \phi(x + h, y - h) + \phi(x + h, y + h)$$

$$= 4\phi + 2h^2 \phi_{xx} + 2h^2 \phi_{yy} + \frac{h^4}{6} \phi_{xxxx} + h^4 \phi_{xxyy} + \frac{h^4}{6} \phi_{yyyy} + O(h^6). \quad (2.3)$$

From Equations (2.2) and (2.3), we have

$$\phi(x - h, y - h) + \phi(x - h, y + h) + \phi(x + h, y - h) + \phi(x + h, y + h)$$

$$+ 4\left[\phi(x + h, y) + \phi(x - h, y) + \phi(x, y - h) + \phi(x, y + h) \right] - 20\phi(x, y)$$

$$= 6h^2 \left(\phi_{xx} + \phi_{yy} \right)(x, y) + \frac{h^4}{2} \left(\phi_{xxxx} + 2\phi_{xxyy} + \phi_{yyyy} \right)(x, y) + O(h^6).$$
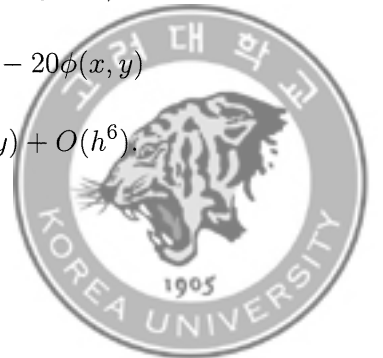
Finally, we have

$$\Delta_c \phi_{ij} = \Delta\phi(x_i, y_j) + \frac{h^2}{12}\Delta^2\phi(x_i, y_j) + O(h^4), \tag{2.4}$$

where $\Delta^2\phi = \Delta(\Delta\phi)$ is the biharmonic operator. For the sake of convenience, we call this approximation *compact nine-point formula* (CNPF).

Note that the standard fourth-order nine-point Laplacian operator Δ_s is defined as

$$\begin{aligned}
\Delta_s \phi_{ij} &= \frac{1}{12h^2}\left(-\phi_{i-2,j} + 16\phi_{i-1,j} - 30\phi_{ij} + 16\phi_{i+1,j} - \phi_{i+2,j}\right) \\
&\quad + \frac{1}{12h^2}\left(-\phi_{i,j-2} + 16\phi_{i,j-1} - 30\phi_{ij} + 16\phi_{i,j+1} - \phi_{i,j+2}\right),
\end{aligned}$$

and its stencil is shown in Figure 2.2(b). In a similar manner, we can derive

$$\Delta_s \phi_{ij} = \Delta\phi(x_i, y_j) + O(h^4).$$

We call this approximation *nine-point formula* (NPF).

In Figure 2.2(a), a second-order five-point stencil is represented for the discrete Laplacian operator $\Delta_d\phi_{ij} = (\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j-1} + \phi_{i,j+1} - 4\phi_{ij})/h^2$, and we define *five-point formula* (FPF) as

$$\Delta_d \phi_{ij} = \Delta\phi(x_i, y_j) + O(h^2).$$

2.2. The Poisson equation

We consider the two-dimensional Poisson equation with a periodic boundary condition,

$$\Delta u(x, y) = f(x, y), \quad (x, y) \in \Omega. \tag{2.5}$$

Now, applying CNPF (2.4) to Equation (2.5), we obtain

$$
\begin{aligned}
\Delta_c u_{ij} &= \Delta u + \frac{h^2}{12}\Delta^2 u + O(h^4) = f + \frac{h^2}{12}\Delta f + O(h^4) \\
&= f_{ij} + \frac{h^2}{12}(\Delta_c f_{ij} + O(h^2)) + O(h^4) \\
&= f_{ij} + \frac{h^2}{12}\Delta_c f_{ij} + O(h^4).
\end{aligned}
\tag{2.6}
$$

Using Equations (2.1) and (2.6), the compact scheme for solving Equation (2.5) is

$$
\begin{aligned}
&\frac{1}{6h^2}[4(u_{i,j+1} + u_{i,j-1} + u_{i+1,j} + u_{i-1,j}) \\
&\quad + (u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1}) - 20u_{ij}] \\
&= f_{ij} + \frac{1}{72}[4(f_{i,j+1} + f_{i,j-1} + f_{i+1,j} + f_{i-1,j}) \\
&\quad + (f_{i+1,j+1} + f_{i+1,j-1} + f_{i-1,j+1} + f_{i-1,j-1}) - 20f_{ij}].
\end{aligned}
\tag{2.7}
$$

For instance, we take $f(x, y) = -8\pi^2 \cos(2\pi x)\cos(2\pi y)$ in the Poisson equation (2.5) and its domain is $\Omega = (0, 1) \times (0, 1)$. Then the exact solution for the equation is

$$u^{ex}(x, y) = \cos(2\pi x)\cos(2\pi y)$$

as shown in Figure 2.3.
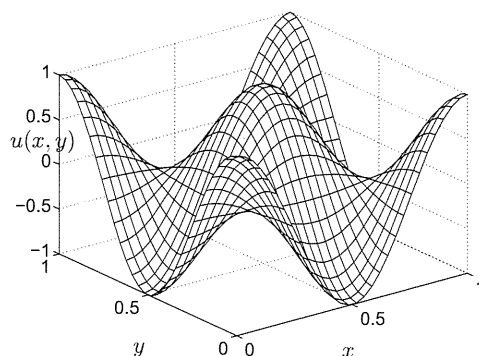
FIGURE 2.3. The exact solution of the Poisson equation.

We denote the error by $e_{ij} := u_{ij} - u_{ij}^{ex}$. The convergence rate is defined as the ratio of successive errors, $\log_2(\|e_h\|/\|e_{h/2}\|)$, where $\|e_h\|$ is the discrete l_2-norm of error function e_h. The numerical convergence tests for Equation (2.7) using the three schemes are performed with increasingly finer grids $h = 1/2^n$, for $n = 3, \cdots, 8$.

Table 2.1 lists the discrete l_2-norm of errors and convergence rates with three different formulas. Using CNPF, we have the fourth-order accuracy in space as we expect from the discretization.

TABLE 2.1. l_2-norm errors and convergence rates for FPF and CNPF

	FPF		CNPF	
h	error	order	error	order
1/8	2.651×10^{-2}		5.065×10^{-4}	
1/16	6.475×10^{-3}	2.034	3.272×10^{-5}	3.952
1/32	1.609×10^{-3}	2.008	2.060×10^{-6}	3.990
1/64	4.018×10^{-4}	2.002	1.289×10^{-7}	3.997
1/128	1.004×10^{-4}	2.001	8.063×10^{-9}	3.999
1/256	2.510×10^{-5}	2.000	5.069×10^{-10}	3.991

2.3. Heat equation

We consider the two-dimensional heat equation with a periodic boundary condition,

$$u_t(x, y, t) = \Delta u(x, y, t), \quad (x, y) \in \Omega, \quad 0 < t \le T. \tag{2.8}$$

Now, applying CNPF (2.4) to Equation (2.8), we obtain

$$
\begin{aligned}
\Delta_c u_{ij} &= \Delta u + \frac{h^2}{12}\Delta^2 u + O(h^4) = u_t + \frac{h^2}{12}\Delta u_t + O(h^4) \\
&= u_t + \frac{h^2}{12}(\Delta_c u_t + O(h^2)) + O(h^4) \\
&= u_t + \frac{h^2}{12}\Delta_c u_t + O(h^4).
\end{aligned} \tag{2.9}
$$

We apply backward time difference to Equation (2.9), then

$$\Delta_c u_{ij}^{n+1} = \frac{u_{ij}^{n+1} - u_{ij}^n}{\Delta t} + \frac{h^2}{12}\frac{\Delta_c u_{ij}^{n+1} - \Delta_c u_{ij}^n}{\Delta t}.$$

By arranging the above equation, we get

$$\frac{1}{\Delta t}u_{ij}^{n+1} - \left(1 - \frac{h^2}{12\Delta t}\right)\Delta_c u_{ij}^{n+1} = \frac{1}{\Delta t}u_{ij}^n + \frac{h^2}{12\Delta t}\Delta_c u_{ij}^n. \tag{2.10}$$

For example, we use the initial condition for heat equation (2.8)

$$u(x, y, 0) = \cos(2\pi x)\cos(2\pi y),$$

in a domain $\Omega = (0, 1) \times (0, 1)$ and the exact solution is

$$u^{ex}(x, y, t) = e^{-8\pi^2 t}\cos(2\pi x)\cos(2\pi y)$$

as shown in Figure 2.4.
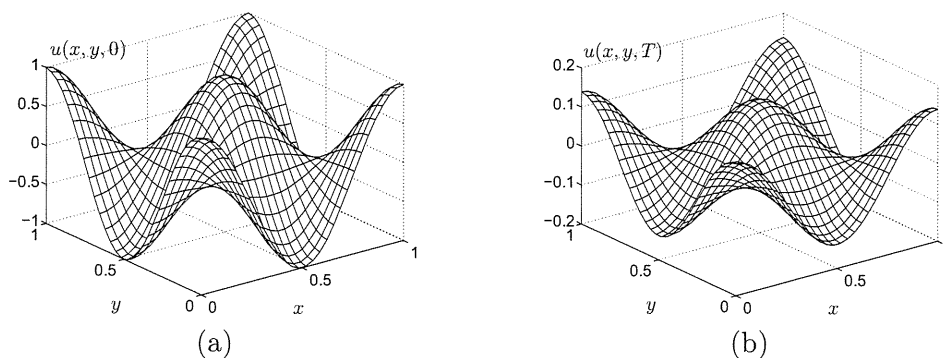
FIGURE 2.4. (a) Initial condition $u(x, y, 0)$ and (b) exact solution $u^{ex}(x, y, T)$ at time $T = 0.025$ for heat equation.

We take convergence tests for Equation (2.10). Table 4.1 lists the discrete l_2-norm of errors and convergence rates with three different formulas. Using CNPF, we have the fourth-order accuracy in space as we expect from the discretization.

TABLE 2.2. l_2-norm errors and convergence rates for FPF and CNPF

h	FPF		CNPF	
	L_2 error	order	L_2 error	order
1/8	1.988×10^{-7}		1.676×10^{-11}	
1/16	5.049×10^{-8}	1.977	1.045×10^{-12}	4.003
1/32	1.268×10^{-8}	1.993	6.522×10^{-14}	4.002
1/64	3.185×10^{-9}	1.993	4.061×10^{-15}	4.005
1/128	8.082×10^{-10}	1.979	2.515×10^{-16}	4.013
1/256	2.138×10^{-10}	1.919	6.301×10^{-17}	1.997

Chapter 3

Numerical method for the Cahn–Hilliard equation

For the sake of convenience, the constant mobility is taken as $M = 1$ throughout this thesis. Then the Cahn–Hilliard equation (1.1) and (1.2) is rewritten as

$$\frac{\partial \phi(\mathbf{x}, t)}{\partial t} = \Delta \mu(\phi(\mathbf{x}, t)), \tag{3.1}$$

$$\mu(\phi(\mathbf{x}, t)) = F'(\phi(\mathbf{x}, t)) - \epsilon^2 \Delta \phi(\mathbf{x}, t), \tag{3.2}$$

where $\Omega \subset \mathbb{R}^2$ is a domain, $\mathbf{x} = (x, y) \in \Omega$, $t > 0$.

3.1. Numerical solution

We derive the fourth-order accurate and practically stable compact finite difference scheme for the Cahn–Hilliard equation (3.1) and (3.2). Beginning with the compact nine-point Laplacian operator for μ_{ij}, we have

$$\begin{aligned}
\Delta_c \mu_{ij} &= \Delta \mu(x_i, y_j) + \frac{h^2}{12} \Delta^2 \mu(x_i, y_j) + O(h^4) \\
&= \phi_t(x_i, y_j) + \frac{h^2}{12} \Delta \phi_t(x_i, y_j) + O(h^4) \\
&= (\phi_t)_{ij} + \frac{h^2}{12} \Delta_c (\phi_t)_{ij} + O(h^4).
\end{aligned} \tag{3.3}$$

Note that Equation (3.1) is used for the second equality in Equation (3.3). We approximate the temporal operator ϕ_t to first-order accuracy by treating it implicitly:

$$\Delta_c \mu_{ij}^{n+1} = \frac{\phi_{ij}^{n+1} - \phi_{ij}^n}{\Delta t} + \frac{h^2}{12} \frac{\Delta_c \phi_{ij}^{n+1} - \Delta_c \phi_{ij}^n}{\Delta t} + O(\Delta t) + O(h^4). \tag{3.4}$$

We apply the linearly stabilized splitting scheme [41] to Equation (3.2):

$$\mu^{n+1} = (\phi^3 - 3\phi)^n + 2\phi^{n+1} - \epsilon^2 \Delta \phi^{n+1}. \tag{3.5}$$

By applying CNPF (2.4) to Equation (3.5), we get

$$\begin{aligned}
\Delta_c \phi_{ij}^{n+1} &= \frac{(\phi^3 - 3\phi)_{ij}^n + 2\phi_{ij}^{n+1} - \mu_{ij}^{n+1}}{\epsilon^2} \\
&\quad + \frac{h^2}{12} \Delta \left(\frac{(\phi^3 - 3\phi)^n + 2\phi^{n+1} - \mu^{n+1}}{\epsilon^2} \right)_{ij} + O(h^4) \\
&= \frac{(\phi^3 - 3\phi)_{ij}^n + 2\phi_{ij}^{n+1} - \mu_{ij}^{n+1}}{\epsilon^2} \\
&\quad + \frac{h^2}{12\epsilon^2} \left(\Delta_c(\phi^3 - 3\phi)_{ij}^n + 2\Delta_c \phi_{ij}^{n+1} - \Delta_c \mu_{ij}^{n+1} \right) + O(h^4).
\end{aligned} \tag{3.6}$$

Finally, from Equation (3.4) and Equation (3.6), we have the fourth-order accurate and practically stable compact finite difference scheme for the Cahn–Hilliard equation:

$$\frac{\phi_{ij}^{n+1}}{\Delta t} + \frac{h^2}{12\Delta t} \Delta_c \phi_{ij}^{n+1} - \Delta_c \mu_{ij}^{n+1} = \frac{\phi_{ij}^n}{\Delta t} + \frac{h^2}{12\Delta t} \Delta_c \phi_{ij}^n, \tag{3.7}$$

$$-\frac{2}{\epsilon^2} \phi_{ij}^{n+1} + \left(1 - \frac{h^2}{6\epsilon^2} \right) \Delta_c \phi_{ij}^{n+1} + \frac{1}{\epsilon^2} \mu_{ij}^{n+1} + \frac{h^2}{12\epsilon^2} \Delta_c \mu_{ij}^{n+1}$$

$$= \frac{1}{\epsilon^2} (\phi^3 - 3\phi)_{ij}^n + \frac{h^2}{12\epsilon^2} \Delta_c (\phi^3 - 3\phi)_{ij}^n. \tag{3.8}$$

3.2. Mass conservation

We verify that the compact scheme inherits the total mass conservation. Taking the inner product to Equation (3.7) with a constant grid function $\mathbf{1}$, we get

$$\left(\phi^{n+1}, \mathbf{1}\right)_h + \frac{h^2}{12}\left(\Delta_c\phi^{n+1}, \mathbf{1}\right)_h - \Delta t\left(\Delta_c\mu^{n+1}, \mathbf{1}\right)_h = \left(\phi^{n+1}, \mathbf{1}\right)_h + \frac{h^2}{12}\left(\Delta_c\phi^n, \mathbf{1}\right)_h.$$

For $\left(\Delta_c\phi^n, \mathbf{1}\right)_h$, we have

$$
\begin{aligned}
\left(\Delta_c\phi^n, \mathbf{1}\right)_h &= h^2 \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \Delta_c\phi_{ij}^n \\
&= h^2 \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \left(\frac{D_x\phi_{i+\frac{1}{2},j}^n - D_x\phi_{i-\frac{1}{2},j}^n}{h} + \frac{D_x\phi_{i,j+\frac{1}{2}}^n - D_x\phi_{i,j-\frac{1}{2}}^n}{h}\right) \\
&= h\sum_{j=1}^{N_y}\left(D_x\phi_{N_x+\frac{1}{2},j}^n - D_x\phi_{\frac{1}{2},j}^n\right) + h\sum_{i=1}^{N_x}\left(D_x\phi_{i,N_y+\frac{1}{2}}^n - D_x\phi_{i,\frac{1}{2}}^n\right) = 0.
\end{aligned}
$$

Here, we have used the periodic boundary condition for ϕ, and $\left(\Delta_c\phi^{n+1}, \mathbf{1}\right)_h = \left(\Delta_c\mu^n, \mathbf{1}\right)_h = 0$ can be proved in a similar manner. Thus, we have the mass conserving property, i.e., $\left(\phi^n, \mathbf{1}\right)_h = \left(\phi^{n+1}, \mathbf{1}\right)_h$.

3.3. Multigrid algorithm

We briefly describe the multigrid method and implementation to solve the resulting system. We represent the discrete Cahn–Hilliard system as

$$L_h(\phi^{n+1}, \mu^{n+1}) = (\xi^n, \psi^n),$$

where the linear operator L_h is defined as

$$
\begin{aligned}
L_h(\phi^{n+1}, \mu^{n+1}) = & \left(\frac{\phi_{ij}^{n+1}}{\Delta t} + \frac{h^2}{12\Delta t}\Delta_c \phi_{ij}^{n+1} - \Delta_c \mu_{ij}^{n+1}, \right. \\
& \left. -\frac{2}{\epsilon^2}\phi_{ij}^{n+1} + \left(1 - \frac{h^2}{6\epsilon^2}\right)\Delta_c \phi_{ij}^{n+1} + \frac{1}{\epsilon^2}\mu_{ij}^{n+1} + \frac{h^2}{12\epsilon^2}\Delta_c \mu_{ij}^{n+1} \right),
\end{aligned}
$$

and the source term is

$$(\xi^n, \psi^n) = \left(\frac{\phi_{ij}^n}{\Delta t} + \frac{h^2}{12\Delta t}\Delta_c \phi_{ij}^n, \frac{1}{\epsilon^2}(\phi^3 - 3\phi)_{ij}^n + \frac{h^2}{12\epsilon^2}\Delta_c(\phi^3 - 3\phi)_{ij}^n \right).$$

3.3.1. Smoothing. Compute $\left(\bar{\phi}_k, \bar{\mu}_k\right)$ by applying ν smoothing procedures to (ϕ_k, μ_k).

$$\left(\bar{\phi}_k, \bar{\mu}_k\right) = \mathrm{SMOOTH}^{\nu}\left(\phi_k, \mu_k, L_h, \xi_k, \psi_k\right)$$

on a mesh grid Ω_k. The SMOOTH^{ν} function means that it performs a SMOOTH relaxation operator with approximations ϕ_k and μ_k, and source terms ξ_k and ψ_k. The superscript ν denotes how many times the given relaxation operator is applied to obtain the updated approximations $\left(\bar{\phi}_k, \bar{\mu}_k\right)$. This relaxation step is evaluated using pointwise Gauss–Seidal iterative methods. One SMOOTH relaxation operator step is completed by solving the system by a 2×2 matrix inversion for each i and j.

3.3.2. V-cycle. One V-cycle step comprises the presmoothing, coarse grid correction, and postsmoothing steps. Please refer to the reference text for additional details and background [13].

$$\left(\phi_k^{n+1,m+1}, \mu_k^{n+1,m+1}\right) = \text{V-cycle}(k, \phi_k^{n+1,m}, \mu_k^{n+1,m}, L_h, \xi_k^n, \psi_k^n, \nu_1, \nu_2)$$

where $\phi_k^{n+1,m+1}$ and $\phi_k^{n+1,m}$ are the approximations of ϕ_k^{n+1} before and after the V-cycle. Next, we define the V-cycle.

Presmoothing

$$(\bar\phi_k^{n+1,m}, \bar\mu_k^{n+1,m}) = \text{SMOOTH}^{\nu_1}(\phi_k^{n+1,m}, \mu_k^{n+1,m}, L_h, \xi_k^n, \psi_k^n).$$

Coarse grid correction

1) Find the defect: $\left(\bar d_{1,k}^m, \bar d_{2,k}^m\right) = (\xi_k^n, \psi_k^n) - L_h\left(\bar\phi_k^{n+1,m}, \bar\mu_k^{n+1,m}\right)$.

2) Restrict the defect: $\bar d_{1,k-1}^m = I_k^{k-1}\bar d_{1,k}^m, \ \bar d_{2,k-1}^m = I_k^{k-1}\bar d_{2,k}^m$.

3) Evaluate approximations $\left(\hat v_{1,k-1}^{n+1,m}, \hat v_{2,k-1}^{n+1,m}\right)$ of the following coarse grid system on Ω_{k-1}: $L_{2h}\left(\hat v_{1,k-1}^{n+1,m}, \hat v_{2,k-1}^{n+1,m}\right) = \left(\bar d_{1,k-1}^m, \bar d_{2,k-1}^m\right)$. If $k > 1$, then we can solve the coarse the grid system using the zero grid functions as initial approximations and the defect functions as source terms

$$\left(\hat v_{1,k-1}^{n+1,m}, \hat v_{2,k-1}^{n+1,m}\right) = \text{V-cycle}\left(k-1, 0, 0, L_{2h}, \bar d_{1,k-1}^m, \bar d_{2,k-1}^m, \nu_1, \nu_2\right).$$

Otherwise, we apply the smoothing procedure to obtain the approximations.

4) Interpolate the correction: $\hat v_{1,k}^{n+1} = I_{k-1}^k \hat v_{1,k-1}^{n+1,m}, \ \hat v_{2,k}^{n+1,m} = I_{k-1}^k \hat v_{2,k-1}^{n+1,m}$.

5) Compute the corrected approximation on Ω_k:

$$\left(\widetilde{\phi}_k^{n+1,m}, \widetilde{\mu}_k^{n+1,m} \right) = \left(\bar{\phi}_k^{n+1,m}, \bar{\mu}_k^{n+1,m} \right) + \left(\hat{v}_{1,k}^{n+1,m}, \hat{v}_{2,k}^{n+1,m} \right).$$

Postsmoothing

$$\left(\phi_k^{n+1,m+1}, \mu_k^{n+1,m+1} \right) = \mathrm{SMOOTH}^{\nu_2} \left(\widetilde{\phi}_k^{n+1,m}, \widetilde{\mu}_k^{n+1,m}, L_h; \xi_k^n, \psi_k^n \right).$$

This completes the description of the V-cycle.

Chapter 4

Numerical results for the Cahn–Hilliard equation

Various numerical experiments are given to demonstrate the fourth-order convergence, non-increase of total energy, mass conservation, linear stability analysis, robustness of the scheme, and evolution up to the steady state. In addition, it is performed to verify that the compact scheme is more robust and efficient than the non-compact fourth-order scheme.

4.1. Convergence test

A numerical convergence test for the three schemes is performed with increasingly finer grids $h = 1/2^n$, for $n = 3$, 4, 5, and 6. The initial state is defined as $\phi(x, y, 0) = 0.1 \cos(2\pi x) \cos(2\pi y)$ in $\Omega = (0, 1) \times (0, 1)$ (Figure 4.1(a)), and Figure 4.1(b) illustrates the numerical solution at $T = 24\Delta t$, where we use $\epsilon = 0.0075$ and $\Delta t = 6 \times 10^{-4}$. We consider a reference solution, because it is generally hard to find the exact solution of the Cahn–Hilliard equation. We define the reference solution ϕ_{ij}^{ref} by the local average of numerical solution on a much finer grid, and then denote the error by $e_{ij} := \phi_{ij} - \phi_{ij}^{ref}$. We use a 1024×1024 mesh grid and FPF for the

reference solution ϕ_{ij}^{ref}. The convergence rate is defined as the ratio of successive errors, $\log_2(\|e_h\|/\|e_{h/2}\|)$, where $\|e_h\|$ is the discrete l_2-norm of error function e_h.
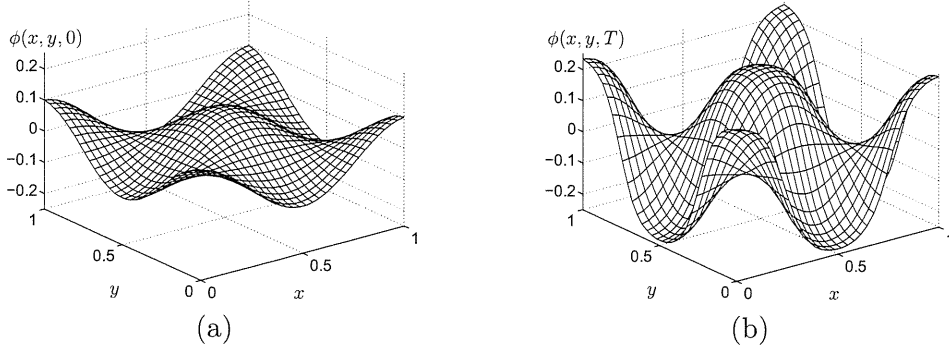

FIGURE 4.1. (a) Initial condition $\phi(x, y, 0)$ and (b) numerical solution $\phi(x, y, T)$ at time $T = 0.0144$

Table 4.1 lists the discrete l_2-norm of errors and convergence rates with different three formula. Using NPF and CNPF, we have the fourth-order accuracy in space as we expect from the discretization.

TABLE 4.1. l_2-norm errors and convergence rates for FPF, NPF, and CNPF

h	FPF error	FPF order	NPF error	NPF order	CNPF error	CNPF order
1/8	1.03×10^{-2}		8.14×10^{-3}		5.02×10^{-3}	
1/16	2.76×10^{-3}	1.90	6.59×10^{-4}	3.63	3.36×10^{-4}	3.90
1/32	7.26×10^{-4}	1.93	4.54×10^{-5}	3.86	2.01×10^{-5}	4.06
1/64	1.83×10^{-4}	1.99	2.31×10^{-6}	4.30	1.27×10^{-6}	3.98

4.2. Non-increase of total energy and conservation of mass

We define the discrete total energy functional by

$$\mathcal{E}^h(\phi^n) = (F(\phi^n), 1)_h + \frac{\epsilon^2}{2}\|\nabla\phi^n\|_e^2.$$

Figure 4.2 demonstrates that the discrete total energy is monotonically decreasing and the mass is conserved. The inscribed small figures show the phase separation at the indicated times. For the numerical test, in $\Omega = (0,1) \times (0,1)$, the initial state is taken as a random perturbation $\phi(x,y,0) = 0.5\text{rand}(x,y)$, where $\text{rand}(x,y)$ is a random value, which is uniformly distributed between -1 and 1. For other parameter, $h = 1/256$, $\Delta t = 0.002$, $T = 3$, and $\epsilon = 0.0038$ are used.
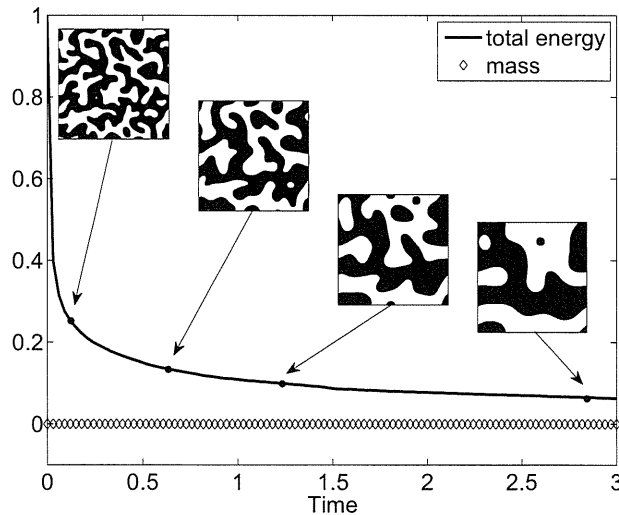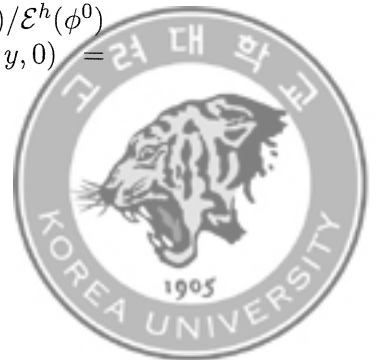

FIGURE 4.2. Non-dimensional discrete total energy $\mathcal{E}^h(\phi^n)/\mathcal{E}^h(\phi^0)$ and mass concentration with the initial condition $\phi(x,y,0) = 0.5\text{rand}(x,y)$

4.3. Linear stability analysis

Let us consider the linear stability analysis for the Cahn–Hilliard equation (1.1) and (1.2)

$$\phi_t = \Delta\left(\phi^3 - \phi - \epsilon^2\Delta\phi\right), \quad \mathbf{x} \in \Omega, \quad t > 0, \tag{4.1}$$

where $\Omega = (0, 2\pi) \times (0, 2\pi)$. We assume that the solution can be expressed by

$$
\begin{aligned}
\phi(x, y, t) \;=\; & \bar{\phi} + \sum_{k_1=1}^{\infty}\sum_{k_2=1}^{\infty} \beta_{k_1 k_2}(t)\cos\left(k_1 x\right)\cos\left(k_2 y\right) \\
& + \sum_{k_1=1}^{\infty}\sum_{k_2=1}^{\infty} \gamma_{k_1 k_2}(t)\sin\left(k_1 x\right)\sin\left(k_2 y\right),
\end{aligned}
\tag{4.2}
$$

where $\bar{\phi}$ is the average of ϕ, and $\beta_{k_1 k_2}(t)$ and $\gamma_{k_1 k_2}(t)$ are amplification factors at wave numbers k_1 and k_2. After linearizing Equation (4.1) and substituting Equation (4.2) into the linearized equation, we have

$$\frac{d\beta_{k_1 k_2}(t)}{dt} = k^2\left(1 - 3\bar{\phi}^2 - \epsilon^2 k^2\right)\beta_{k_1 k_2}(t), \tag{4.3}$$

where we denote $k^2 = k_1^2 + k_2^2$. We only consider $\beta_{k_1 k_2}(t)$ because the same ordinary differential equation holds for $\gamma_{k_1 k_2}(t)$. The solution of Equation (4.3) is $\beta_{k_1 k_2}(t) = \beta_{k_1 k_2}(0)\exp(\eta_{k_1 k_2} t)$, where $\eta_{k_1 k_2} = k^2(1 - 3\bar{\phi}^2 - \epsilon^2 k^2)$ is the growth rate. The numerical growth rate is defined as $\widetilde{\eta}_{k_1 k_2} = \log(\|\phi^m\|_\infty/\|\phi^0\|_\infty)/(m\Delta t)$. We take the initial condition $\phi(x, y, 0) = 0.01\cos(k_1 x)\cos(k_2 y)$ with $m = 100$, $\Delta t = 10^{-8}$, $h = \pi/256$, and $\epsilon = 0.03$. Figures 4.3(a) and (b) show the numerical growth rate $\widetilde{\eta}_{k_1 k_2}$ versus the wave numbers k_1 and k_2 for the Cahn–Hilliard and linearized Cahn–Hilliard equations, respectively. Open and closed circles correspond to the solutions
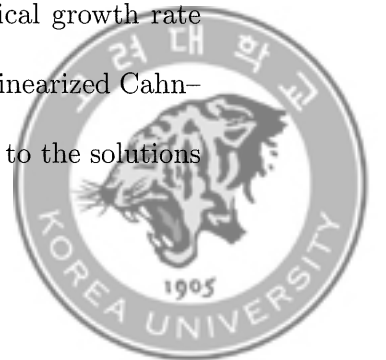
from the linear stability analysis and CNPF, respectively. The numerical results are

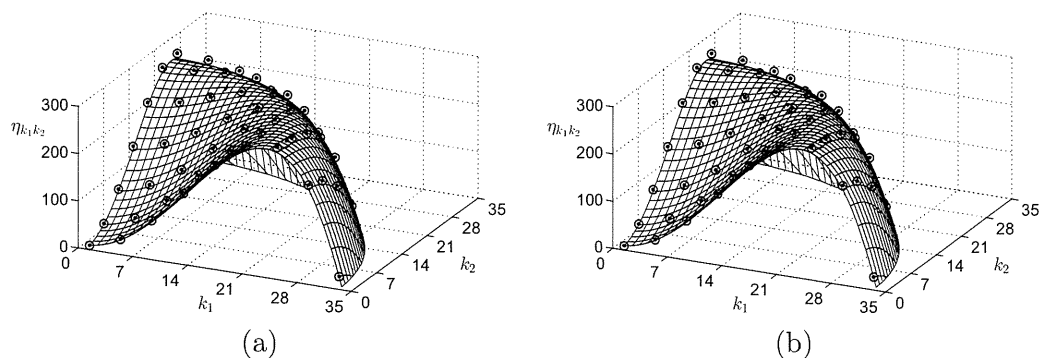in good agreement with the analytic solutions from the linear stability analysis.

FIGURE 4.3. Growth rate versus the wave numbers k_1 and k_2 for the (a) CH and (b) linearized CH equations

4.4. Stability of the proposed scheme

We demonstrate a practical stability of the scheme through a numerical experiment with spinodal decomposition of a binary mixture. In the simulation, the initial condition is taken as $\phi(x, y, 0) = 0.5\text{rand}(x, y)$ in $\Omega = (0, 1) \times (0, 1)$. Note that the maximum amplitude is 0.5 at the initial time. For numerical parameters, $h = 1/128$ and $\epsilon = 0.0113$ are used and different time step $\Delta t = 0.01$, 10, and 10000 are employed. In Figure 4.4, we illustrate the evolutions after fifteen time iterations. As the numerical results, the maximum amplitudes are bounded, and the numerical solutions do not blow up. Therefore, our proposed scheme is stable regardless of the time step size.

(a) $\Delta t = 0.01$ (b) $\Delta t = 10$ (d) $\Delta t = 10000$
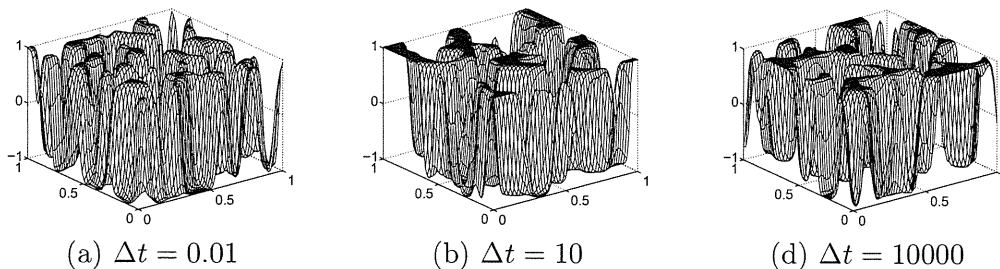
FIGURE 4.4. Evolutions with different time step $\Delta t = 0.01$, 10, and 10000

4.5. Steady state

We examine the evolution of a random perturbation up to the steady state. The initial condition is taken to be $\phi(x, y, 0) = 0.01\text{rand}(x, y)$ in $\Omega = (0, 1) \times (0, 1)$. We then take the simulation parameters as $\epsilon = 0.0075$, $h = 1/256$, and $\Delta t = 10h^2$. We stop the numerical computations when the discrete l_2-norm of the difference between $(n + 1)$th and nth step solutions becomes less than 10^{-9}, i.e., $\|\phi^{n+1} - \phi^n\| \leq 10^{-9}$. Figure 4.5 shows the snapshots of filled contour of the concentration ϕ. We observe that the randomly perturbed concentration ϕ evolves to a complex interconnected pattern. After a long time evolution, a numerical equilibrium state is reached.
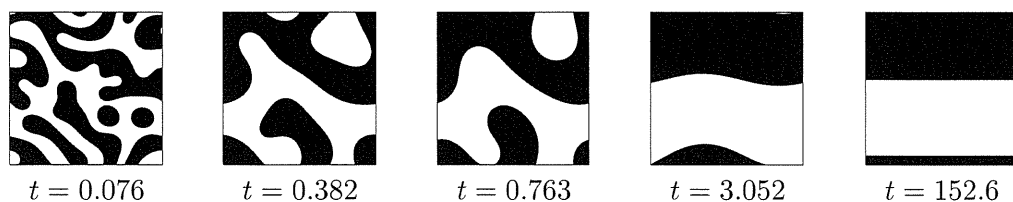

| $t = 0.076$ | $t = 0.382$ | $t = 0.763$ | $t = 3.052$ | $t = 152.6$ |

FIGURE 4.5. Evolution of ϕ up to the steady state time $t = 152.6$. The times are shown below each figure.

4.6. Comparison of schemes

To show the superiority of CNPF, we compare the evolution results from CNPF and FPF, and list the computational times for the three methods. The initial condition is given as

$$\phi(x, y, 0) = \begin{cases} 1 & \text{if } 0.2 < x < 3.8 \text{ and } 0.4 < y < 0.6, \\ -1 & \text{otherwise} \end{cases} \tag{4.4}$$

in $\Omega = (0, 4) \times (0, 1)$. Here, a mesh grid 256×64, $\epsilon = 0.015$, $\Delta t = 0.0005$, and $T = 10$ are used. We define the reference solution by numerical solutions, using FPF, on a finer mesh 1024×256. In Figure 4.6, we illustrate evolutions by CNPF (circles) and FPF (dashed line) with the reference solutions (solid line) at $t = 0$, 2, 6, and 10. Table 4.2 lists CPU times of the three schemes to $T = 10$. Although CNPF has a slight difference of CPU time than FPF, it has higher accuracy compared to FPF. Furthermore, NPF needs more V-cycle iterations than CNPF to reach the V-cycle tolerance, and it results in the increment of CPU time.
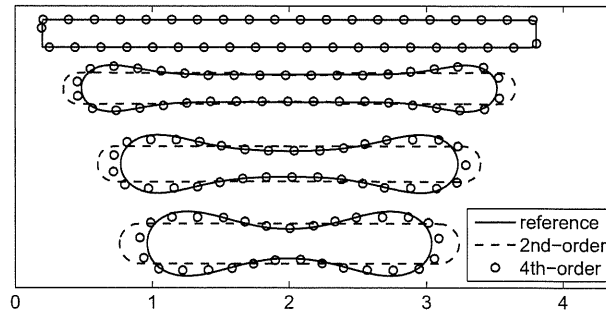

FIGURE 4.6. Evolutions for FPF and CNPF with a mesh grid 256×64. Note that the reference solution is defined by use much more finer mesh 1024×256. From top to bottom, times are $t = 0$, 2, 6, and 10.

TABLE 4.2. CPU time (sec) for FPF, NPF, and CNPF

FPF	NPF	CNPF
1819	3095	2218

4.7. Comparison between CNPF and NPF

We compare the numerical convergence of two formula, CNPF and NPF. For the numerical test, we take the initial condition as $\phi(x, y, 0) = 0.1 \cos(2\pi x) \cos(2\pi y)$ in $\Omega = (0, 1) \times (0, 1)$. For other parameter, we use $h = 1/64$ and $\epsilon = 0.015$. We count the number of V-cycle until the maximum value of residual error is less than 10^{-10}. Figure 4.7 plots the numbers of V-cycle for one time iteration versus Δt. From the results, we can observe that CNPF requires less V-cycle iterations than NPF for all time step sizes.
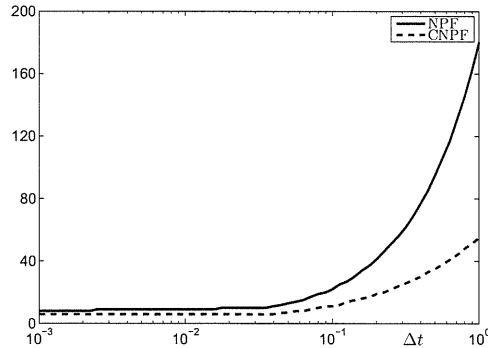

FIGURE 4.7. V-cycle number with different time step Δt

Chapter 5

Conclusion

We proposed the fourth-order accurate and practically stable compact finite difference method for the Cahn–Hilliard equation. The compact nine-point formula (CNPF) and linearly stabilized splitting scheme were presented for the equation. We described the multigrid algorithm to solve the discrete Cahn–Hilliard system.

Numerical experiments were performed to demonstrate the fourth-order accuracy, decreasing of total energy, mass conservation, and practical stability. Also, to verify the superiority of proposed scheme, we compared the standard nine-point formula (NPF) with CNPF. Since NPF needs more V-cycle iterations than CNPF to reach the tolerance, the computational time of CNPF was less than that of NPF. NPF had a disadvantage due to the wide stencil compared to CNPF.

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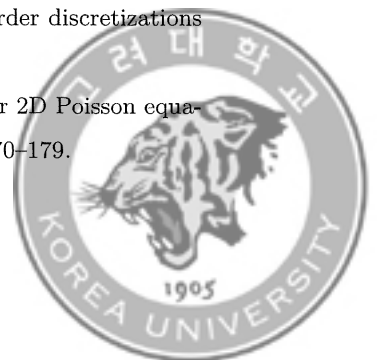
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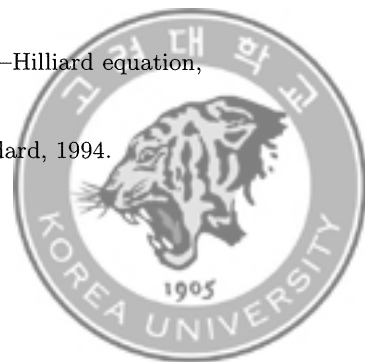
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