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Numerical Analysis of First and Second Order Unconditional Energy Stable Schemes for Nonlocal Cahn-Hilliard and Allen-Cahn Equations

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To the Graduate Council:

I am submitting herewith a dissertation written by Zhen Guan entitled "Numerical Analysis of First and Second Order Unconditional Energy Stable Schemes for Nonlocal Cahn-Hilliard and Allen-Cahn Equations." I have examined the final electronic copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Mathematics.

Steven M. Wise, Major Professor

We have read this dissertation and recommend its acceptance:

Grozdena Todorova, Vasilios Alexiades, Yanfei Gao

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(Original signatures are on file with official student records.)

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A Thesis Presented for

The Doctor of Philosophy

Degree

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Zhen Guan

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I dedicated this dissertation to all people who have provided their guidance and help throughout my research, including members of my committee, Steven M. Wise, Grozdena Todorova, Vasilios Alexiades and Yanfei Gao. And many other faculties and staffs who have provided me with excellent level of support in my Ph.D program at the University of Tennessee, Knoxville. Also, I would like to dedicate this work to my parents Hailong Guan and Jianmin Zhao. Their continuous support gave me the strength to realize my dream.

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Abstract

This PhD dissertation concentrates on the numerical analysis of a family of fully discrete, energy stable schemes for nonlocal Cahn-Hilliard and Allen-Cahn type equations, which are integro-partial differential equations (IPDEs). These two IPDEs – along with the evolution equation from dynamical density functional theory (DDFT), which is a generalization of the nonlocal Cahn-Hilliard equation – are used to model a variety of physical and biological processes such as crystallization, phase transformations, and tumor growth. This dissertation advances the computational state-of-the-art related to this field in the following main contributions: (I) We propose and analyze a family of two-dimensional unconditionally energy stable schemes for these IPDEs. Specifically, we prove that the schemes are (a) uniquely solvable, independent of time and space step sizes; (b) energy stable, independent of time and space step sizes; and (c) convergent, provided the time step sizes are sufficiently small. (II) We develop a highly efficient solver for schemes we propose. These schemes are semi-implicit and contain nonlinear implicit terms, which makes numerical solutions challenging. To overcome this difficulty, a nearly-optimally efficient nonlinear multigrid method is employed. (III) Via our numerical methods, we are able to simulate crystal nucleation and growth phenomena, with arbitrary crystalline anisotropy, with properly chosen parameters for nonlocal Cahn-Hilliard equation, in a very efficient and straightforward way. To our knowledge these contributions do not exist in any form in any of the previous works in the literature.

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Chapter 1

Introduction

1.1 The Nonlocal Cahn-Hilliard and Allen-Cahn Equations

In this section we define the two-dimensional integro-partial differential equation (IPDE) problems we are studying. First we define some notations that we are going to use for the rest of the dissertation. Let $\Omega = [0, L_{x_1}] \times [0, L_{x_2}] \subset \mathbb{R}^2$ be a two-dimensional-rectangle, and set $\Omega_T = \Omega \times [0, T]$. Define

$$C_p^m(\Omega) = \left\{ f \in C^m \left(\mathbb{R}^2\right) \;\middle|\; f \text{ is } \Omega - \text{periodic} \right\},$$

where m is a positive integer. Set $C_p^\infty(\Omega) = \bigcap_{m=1}^{\infty} C_p^m(\Omega)$. Likewise, for any $1 \le q < \infty$, define

$$L_p^q(\Omega) = \left\{ f \in L_{loc}^q \left(\mathbb{R}^2\right) \;\middle|\; f \text{ is } \Omega - \text{periodic} \right\}.$$

Of course, $L^q(\Omega)$ and $L_p^q(\Omega)$ can be identified in a natural way. Specifically, for any $\phi \in L^q(\Omega)$, ϕ can also be viewed as a function in $L_p^q(\Omega)$ by a canonical periodic extension. On the other hand, for any $\phi \in L_p^q(\Omega)$, the restriction $\phi|_\Omega$ is in $L^q(\Omega)$. As in [37], we define $H_p^m(\Omega)$ to be the completion of $C_p^\infty(\Omega)$ in the Sobolev norm $\| \cdot \|_{H^m}$.

We need the notion of a convolution of functions belonging periodic function spaces. Given $\phi\ ,\psi \in L^2_p(\Omega)$, the *circular convolution* $\psi * \phi$ is defined as

$$(\psi * \phi)(\mathbf{x}) := \int_\Omega \psi(\mathbf{y})\,\phi(\mathbf{x}-\mathbf{y})\,d\mathbf{y} = \int_\Omega \psi(\mathbf{x}-\mathbf{y})\,\phi(\mathbf{y})\,d\mathbf{y}\ , \quad \forall \mathbf{x} \in \Omega. \tag{1.1}$$

Clearly $\varphi * 1 = \int_\Omega \varphi(\mathbf{x})\,d\mathbf{x}$ is a constant.

Similar to [6, 7], the periodic nonlocal Cahn-Hilliard (nCH) problem on Ω_T is defined as follows: given $\phi(\,\cdot\,,0) = \phi_0$, where ϕ_0 is Ω-periodic, find $\phi(\mathbf{x},t)$ and $w(\mathbf{x},t)$ such that

$$\begin{cases} \partial_t\phi = \Delta w, \\ \quad w = \phi^3 + \gamma_c\phi - \gamma_e\phi + (J*1)\phi - J*\phi, \\ \qquad \phi(\,\cdot\,,t) \text{ and } w(\,\cdot\,,t) \text{ are } \Omega\text{-periodic for any } t\in[0,T], \end{cases} \tag{1.2}$$

where γ_c and γ_e are non-negative constants. The function $J : \mathbb{R}^2 \to \mathbb{R}$ is called the *correlation function* and is assumed to satisfy the following three conditions:

J1) $J = J_c - J_e$, where $J_c,\ J_e \in C_p^\infty(\Omega)$ are non-negative.

J2) J_c and J_e are even, *i.e.*, $J_\alpha(x_1,x_2) = J_\alpha(-x_1,x_2) = J_\alpha(x_1,-x_2)$, for all $x_1, x_2 \in \mathbb{R}$, $\alpha = c,\ e$.

J3) $\int_\Omega J(\mathbf{x})\,d\mathbf{x} > 0$.

By condition (J3) and the definition of periodic convolution, $J * 1 = \int_\Omega J(\mathbf{x})d\mathbf{x}$ is a positive constant. For the moment the IPDE (1.2) may be viewed as a model for phase transformations in a material. The use of periodic boundary conditions is justified provided one is interested in the phase dynamics of a given material far away from any physical boundary.

Similar to [5, 8] the periodic nonlocal Allen-Cahn (nAC) problem on Ω_T is defined as follows: given $\phi(\,\cdot\,,0) = \phi_0$, where ϕ_0 is Ω-periodic, find $\phi(\mathbf{x},t)$ and $w(\mathbf{x},t)$ such that

$$\begin{cases} \partial_t \phi = -w, \\ w = \phi^3 + \gamma_c \phi - \gamma_e \phi + (J * 1)\phi - J * \phi, \\ \quad \phi(\,\cdot\,, t) \text{ and } w(\,\cdot\,, t) \text{ are } \Omega\text{-periodic for any } t \in [0, T]. \end{cases} \tag{1.3}$$

Observe that the nCH equation (1.2) can be rewritten as

$$\partial_t \phi = \nabla \cdot (a(\phi)\nabla\phi) - (\Delta J) * \phi \ , \tag{1.4}$$

where

$$a(\phi) = 3\phi^2 + \gamma_c - \gamma_e + J * 1. \tag{1.5}$$

We refer to $a(\phi)$ as the diffusive mobility, or just the diffusivity. To make Eq. (1.2) positive diffusive (and non-degenerate), therefore, we require

$$\gamma_c - \gamma_e + J * 1 =: \gamma_0 > 0 \ , \tag{1.6}$$

in which case $a(\phi) > 0$. We will assume that (1.6) holds in the sequel.

In [6, 7, 8] P. Bates, J. Han and G. Zhao proved the well-posedness of the IPDEs (1.2) and (1.3) with Dirichlet and Neumann boundary conditions. By a simple extension of the methods in [6, 7], one can show that, for any $T > 0$, a classical periodic solution $\phi(\mathbf{x}, t)$ for Eq. (1.2) exists and $\phi \in C_p^{2+\beta, \frac{2+\beta}{2}}(\Omega_T)$ if the initial data satisfy $\phi(\mathbf{x}, 0) \in C_p^{2+\beta}(\Omega)$ for any $\beta > 0$*. In some applications the initial data may not have sufficient regularity to justify the existence a classical solution. Therefore we also define the weak solution of Eq. (1.2) as in [6, 7].

*Note that, for the sake of brevity, we did not specifically define $C_p^q(\Omega)$, where q is a positive rational number, or for that matter $C_p^{\alpha,\beta}(\Omega_T)$. But the definitions but these spatially periodic function spaces can be established straightforwardly.

Definition 1.1.1. *A weak solution of Eq. (1.2) is a pair of* (ϕ, w)

$$\phi(x,t) \in C\left([0,T], L^2_p(\Omega)\right) \cap L^\infty\left([0,T], L^\infty_p(\Omega)\right), \tag{1.7}$$

$$w(x,t) \in L^2\left([0,T], H^1_p(\Omega)\right), \tag{1.8}$$

$$\partial_t\phi(x,t) \in L^2\left([0,T], H^{-1}_p(\Omega)\right) \tag{1.9}$$

such that

$$\langle \partial_t\phi, \mu\rangle + (\nabla w, \nabla\mu) = 0, \quad \forall\mu \in H^1_p(\Omega), \tag{1.10}$$

$$(w,\chi) - \left(\phi^3 + (\gamma_c - \gamma_e + J * 1)\phi, \chi\right) + (J * \phi, \chi) = 0, \quad \forall\chi \in L^2_p(\Omega), \tag{1.11}$$

for a.e. $0 \le t \le T$*. Here* $\langle\cdot,\cdot\rangle$ *is the dual pairing between the dual space* $H^{-1}_p(\Omega) := \left(H^1_p(\Omega)\right)^*$ *and* $H^1_p(\Omega)$.

We refer the reader to the literature [6, 7, 8] regarding the details of the well-posedness of the periodic nAC problem.

1.2 The Nonlocal Cahn-Hilliard Type Energy

1.2.1 The Definition of Nonlocal Cahn-Hilliard Type Energy

The nCH and nAC equations may derived as gradient flows with respect to some nonlocal energy. To see this, consider the following energy [6, 7, 8]: for any $\phi \in L^4_p(\Omega)$ define

$$E(\phi) = \frac{1}{4}\|\phi\|^4_{L^4(\Omega)} + \frac{\gamma_c}{2}\|\phi\|^2_{L^2(\Omega)} - \frac{\gamma_e}{2}\|\phi\|^2_{L^2(\Omega)} + \frac{J*1}{2}\|\phi\|^2_{L^2(\Omega)} - \frac{1}{2}(\phi, J*\phi)_{L^2(\Omega)}, \tag{1.12}$$

where γ_c, $\gamma_e \ge 0$ are constants and the correlation function J satisfies conditions (J1) – (J3). We refer to E as the *free energy* or just the energy. The expression in (1.12) is equivalent to

$$E(\phi) = \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{\gamma_c - \gamma_e}{2}\phi^2 + \frac{1}{4}\int_\Omega J(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x}. \tag{1.13}$$

We have the following lemma regarding the coercivity of the energy.

Lemma 1.2.1. *There exists a non-negative constant C_0 such that for all $\phi \in L^4_p(\Omega)$, $E(\phi) + C_0 \geq 0$. More specifically,*

$$\frac{1}{8}\|\phi\|^4_{L^4} \leq E(\phi) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right)\right)^2}{2}|\Omega|, \tag{1.14}$$

$$\frac{1}{2}\|\phi\|^2_{L^2} \leq E(\phi) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right) - 1\right)^2}{4}|\Omega|. \tag{1.15}$$

If $\gamma_e = 0$, then $E(\phi) \geq 0$ for all $\phi \in L^4_p(\Omega)$.

Proof. By the symmetric property of J

$$
\begin{aligned}
&\int_\Omega \left\{ \frac{1}{4} \int_\Omega J(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x} \\
=&\int_\Omega \left\{ \frac{1}{4} \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} - \frac{1}{4} \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x} \\
=&\frac{1}{4} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
&- \frac{1}{4} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} - \frac{1}{4} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
&+ \frac{1}{2} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi(\mathbf{x}) \phi(\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
=&\frac{1}{4} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
&- \frac{1}{2} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} + \frac{1}{2} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi(\mathbf{x}) \phi(\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
=&\frac{1}{4} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
&+ \frac{1}{2} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} + \frac{1}{2} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi(\mathbf{x}) \phi(\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
&- \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} \\
=&\frac{1}{4} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} + \frac{1}{4} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
&- \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} \\
\geq& - \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} \ . \qquad (1.16)
\end{aligned}
$$

By the definition of periodic convolution

$$
\int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} = \int_\Omega \phi^2(\mathbf{x}) \left\{ \int_\Omega J_e(\mathbf{x}-\mathbf{y}) d\mathbf{y} \right\} d\mathbf{x} = \int_\Omega \left(J_e * 1\right) \phi^2(\mathbf{x}) d\mathbf{x} \ . \qquad (1.17)
$$

With two identities above we have

$$
\int_\Omega \left\{ \frac{1}{4} \int_\Omega J(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x} \geq - \int_\Omega \left(J_e * 1\right) \phi^2(\mathbf{x}) d\mathbf{x} \ . \qquad (1.18)
$$

Thus by the definition of $E(\phi)$

$$E(\phi) \geq \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{\gamma_c - \gamma_e - 2(J_e * 1)}{2}\phi^2 \right\} d\mathbf{x}. \tag{1.19}$$

Also notice identities

$$\frac{1}{8}\phi^4 \leq \frac{1}{4}\phi^4 + \frac{c}{2}\phi^2 + \frac{c^2}{2}, \tag{1.20}$$

$$\frac{1}{2}\phi^2 \leq \frac{1}{4}\phi^4 + \frac{c}{2}\phi^2 + \frac{(c-1)^2}{4}, \tag{1.21}$$

where $c \in R$ is a constant. Therefore

$$\frac{1}{8}\int_\Omega \phi^4 d\mathbf{x} \leq E(\phi) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right)\right)^2}{2}|\Omega|, \tag{1.22}$$

$$\frac{1}{2}\int_\Omega \phi^2 d\mathbf{x} \leq E(\phi) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right) - 1\right)^2}{4}|\Omega|. \tag{1.23}$$

□

Remark 1.2.1. *Observe that the energy is rather weak. Specifically, the energy is not powerful enough to coerce the* H^1 *norm of* ϕ.

Lemma 1.2.2. *The energy (1.12) can be written as the difference of convex functionals,* i.e, $E = E_c - E_e$, *where*

$$E_c(\phi) = \frac{1}{4}\left\|\phi\right\|_{L^4(\Omega)}^4 + \frac{\gamma_c}{2}\left\|\phi\right\|_{L^2(\Omega)}^2 + (J_c * 1)\left\|\phi\right\|_{L^2(\Omega)}^2, \tag{1.24}$$

$$E_e(\phi) = \frac{\gamma_e}{2}\left\|\phi\right\|_{L^2(\Omega)}^2 + \frac{J_c * 1}{2}\left\|\phi\right\|_{L^2(\Omega)}^2 + \frac{J_e * 1}{2}\left\|\phi\right\|_{L^2(\Omega)}^2 + \frac{1}{2}\left(\phi, J * \phi\right)_{L^2(\Omega)} \tag{1.25}$$

Proof. Notice that by the symmetric property of J and the definition of periodic convolution

$$
\begin{aligned}
&\int_\Omega \left\{ \frac{1}{4} \int_\Omega J(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x} \\
=& \int_\Omega \left\{ \frac{1}{4} \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} - \frac{1}{4} \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x} \\
=& \frac{1}{4} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} + \frac{1}{4} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
& - \frac{1}{2} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi(\mathbf{x}) \phi(\mathbf{y}) d\mathbf{y} d\mathbf{x} - \frac{1}{4} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
=& \frac{1}{2} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} - \frac{1}{2} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi(\mathbf{x}) \phi(\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
& - \frac{1}{4} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
=& - \frac{1}{2} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} - \frac{1}{2} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi(\mathbf{x}) \phi(\mathbf{y}) d\mathbf{y} d\mathbf{x} \\
& + \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} - \frac{1}{4} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
=& - \frac{1}{4} \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) + \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} - \frac{1}{4} \int_\Omega \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} d\mathbf{x} \\
& + \int_\Omega \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \phi^2(\mathbf{x}) d\mathbf{y} d\mathbf{x} \\
=& - \frac{1}{4} \int_\Omega \left\{ \int_\Omega J_c(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) + \phi(\mathbf{y})\right)^2 d\mathbf{y} + \int_\Omega J_e(\mathbf{x}-\mathbf{y}) \left(\phi(\mathbf{x}) - \phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x} \\
& + \int_\Omega \left(J_c * 1\right) \phi(\mathbf{x})^2 d\mathbf{x}.
\end{aligned}
\tag{1.26}
$$

Therefore $E(\phi)$ can be rewritten as

$$E(\phi) = E_c(\phi) - E_e(\phi), \tag{1.27}$$

where

$$E_c(\phi) = \int_\Omega \left\{ \frac{1}{4}\phi^4 + \frac{2(J_c * 1) + \gamma_c}{2}\phi^2 \right\} d\mathbf{y} \tag{1.28}$$

and

$$
\begin{aligned}
E_e(\phi) = & -\frac{1}{4}\int_\Omega\int_\Omega J_c(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})+\phi(\mathbf{y})\right)^2 d\mathbf{y}\mathbf{x} \\
& -\frac{1}{4}\int_\Omega\int_\Omega J_e(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})-\phi(\mathbf{y})\right)^2 d\mathbf{y}d\mathbf{x} \\
& +\int_\Omega \frac{\gamma_e}{2}\phi(\mathbf{x})^2 d\mathbf{x}. \qquad (1.29)
\end{aligned}
$$

We now show that these functionals are convex. Calculating the first variation of $E_c(\phi)$ yields

$$
\left.\frac{dE_c}{ds}(\phi+s\psi)\right|_{s=0} = \left(\phi^3+(2(J_c*1)+\gamma_c)\,\phi,\psi\right)_{L^2}. \qquad (1.30)
$$

Calculating the second variation of $E_c(\phi)$ reveals

$$
\left.\frac{d^2E_c}{ds^2}(\phi+s\psi)\right|_{s=0} = \left(2\phi^2+(2(J_c*1)+\gamma_c)\,,1\right)_{L^2} \geq 0, \qquad (1.31)
$$

which prove $E_c(\phi)$ is convex. Similarly, calculating the first variation of $E_e(\phi)$ yields

$$
\begin{aligned}
\left.\frac{dE_e}{ds}(\phi+s\psi)\right|_{s=0} = & \left(\gamma_e\phi,\psi\right)_{L^2} \\
& +\frac{1}{2}\int_\Omega\int_\Omega J_c(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})+\phi(\mathbf{y})\right)\left(\psi(\mathbf{x})+\psi(\mathbf{y})\right) d\mathbf{y}d\mathbf{x} \\
& +\frac{1}{2}\int_\Omega\int_\Omega J_e(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})-\phi(\mathbf{y})\right)\left(\psi(\mathbf{x})-\psi(\mathbf{y})\right) d\mathbf{y}d\mathbf{x}\,. \qquad (1.32)
\end{aligned}
$$

Together with the symmetric property of J and the definition of periodic convolution Eq. (1.32) yields

$$\begin{aligned}\frac{dE_e}{ds}(\phi+s\psi)\bigg|_{s=0} &= (\gamma_e\phi,\psi)_{L^2} \\ &\quad + \int_\Omega\int_\Omega J_c(\mathbf{x}-\mathbf{y})\phi(\mathbf{x})\psi(\mathbf{x})d\mathbf{y}d\mathbf{x} \\ &\quad + \int_\Omega\int_\Omega J_c(\mathbf{x}-\mathbf{y})\phi(\mathbf{y})\psi(\mathbf{x})d\mathbf{y}d\mathbf{x} \\ &\quad + \int_\Omega\int_\Omega J_e(\mathbf{x}-\mathbf{y})\phi(\mathbf{x})\psi(\mathbf{x})d\mathbf{y}d\mathbf{x} \\ &\quad - \int_\Omega\int_\Omega J_e(\mathbf{x}-\mathbf{y})\phi(\mathbf{y})\psi(\mathbf{x})d\mathbf{y}d\mathbf{x} \\ &= \left((\gamma_e + J_c * 1 + J_e * 1)\,\phi,\psi\right)_{L^2} + \left((J_c - J_e) * \phi,\psi\right)_{L^2} \ . \end{aligned} \tag{1.33}$$

Calculating the second variation of $E_e(\phi)$ yields

$$\begin{aligned}\frac{d^2E_e}{ds^2}(\phi+s\psi)\bigg|_{s=0} &= (\gamma_e\psi,\psi)_{L^2} + \frac{1}{2}\int_\Omega\int_\Omega J_c(\mathbf{x}-\mathbf{y})\left(\psi(\mathbf{x})+\psi(\mathbf{y})\right)^2 d\mathbf{y}d\mathbf{x} \\ &\quad + \frac{1}{2}\int_\Omega\int_\Omega J_e(\mathbf{x}-\mathbf{y})\left(\psi(\mathbf{x})-\psi(\mathbf{y})\right)^2 d\mathbf{y}d\mathbf{x} \\ &\geq 0 \ , \end{aligned} \tag{1.34}$$

which prove $E_e(\phi)$ is also convex. □

Remark 1.2.2. *The convex splitting decomposition of E is not unique, but the specific one presented in Lem. 1.2.2 is the most useful for our purposes. In particular, the fact that the nonlocal part of the energy can be pushed to the concave part of the energy, E_e – even though in some ways it would be more natural to group it with the convex part, E_c – will be exploited in the numerical schemes.*

A more general form of the free energy (1.13) is, of course,

$$E(\phi) = \int_\Omega \left\{ F(\phi) + \frac{1}{4}\int J(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})-\phi(\mathbf{y})\right)^2 d\mathbf{y} \right\} d\mathbf{x} \ . \tag{1.35}$$

In this context, F is often called the *homogeneous free energy density*, and the corresponding integral, $\int_\Omega F(\phi)\,d\mathbf{x}$, is called the *homogeneous free energy*. The term $\frac{1}{4}J(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})-\phi(\mathbf{y})\right)^2\,d\mathbf{y}$ is called the *gradient free energy density*, and its corresponding integral,

$$\frac{1}{4}\int_\Omega\int_\Omega J(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})-\phi(\mathbf{y})\right)^2 d\mathbf{y}d\mathbf{x},$$

is often referred to as the *gradient free energy*. A common modeling practice is to choose a symmetric quartic potential for homogeneous term:

$$F(\phi)=\frac{1}{4}\left(\phi^2+(\gamma_c-\gamma_e)\right)^2+C$$

where C is a constant. In this case, the energy (1.13) can clearly be derived from the more general (1.35). In the case that $\gamma_c=0$, $\gamma_e=1$ and $C=0$, $F(\phi)$ becomes a widely used quartic double-well potential, as shown in Fig. 1.1.

1.2.2 The Dissipation of Nonlocal Cahn-Hilliard Type Energy

We now define the *chemical potential* w relative to the energy (1.13) for Eq. (1.2) and Eq. (1.3). Denote $\delta_\phi E$ to be the variational derivative of functional $E(\phi)$ with respect to ϕ, then

$$w:=\delta_\phi E=\phi^3+\gamma_c\phi-\gamma_e\phi+(J*1)\phi-J*\phi. \tag{1.36}$$

The chemical potential w can also be divided into two parts. The variational derivative of the homogeneous energy is referred to as the homogeneous part of the chemical potential; the variational derivative of gradient energy is referred to as the gradient part of the chemical potential. The conserved gradient equation relative to the energy (1.13), – in other words, the H^{-1} gradient flow of the energy (1.13) [6, 7]

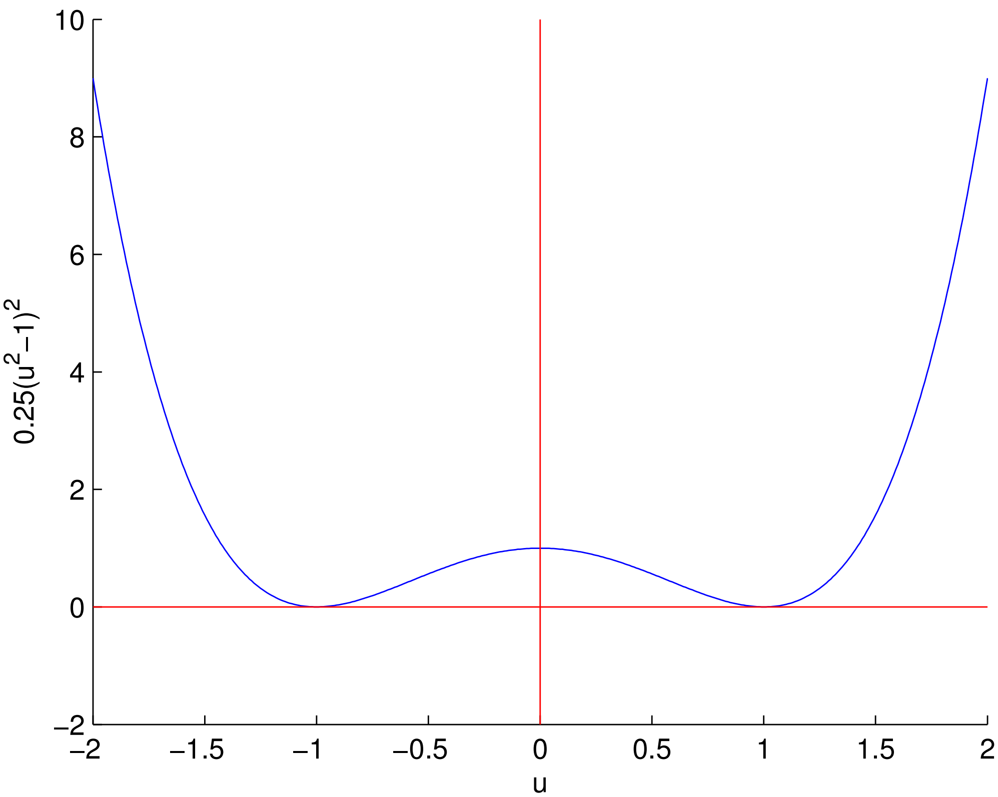


Figure 1.1: A typical quartic double-well homogeneous free energy density, $F(u)$. The minima of F are found at $u = \pm 1$, which represent the energetically preferred states.

– is expressed simply as

$$\partial_t \phi = \Delta w, \tag{1.37}$$

which yields the nonlocal Cahn-Hilliard (nCH) equation (1.2). Testing Eq. (1.37) with 1 yields

$$\frac{d}{dt} (\phi, 1)_{L^1} = (\partial_t \phi, 1)_{L^1} = (\Delta w, 1)_{L^1} = 0 \ , \tag{1.38}$$

thus $\int_\Omega \phi(\mathbf{x}, t) dx = \int_\Omega \phi(\mathbf{x}, 0) dx$ for any $0 \le t \le T$. In other words, Eqs. (1.2) and (1.37) are mass conserving. More importantly, classical periodic solutions of (1.2) dissipate the energy (1.13) at the following rate:

$$d_t E(\phi) = - \|\nabla w\|^2_{L^2(\Omega)} \,. \tag{1.39}$$

Weak solutions of Eq. (1.2) still dissipate the energy E (1.13), but the rate of dissipation is presented in weak form as

$$E\left(\phi(\cdot, s)\right) + \int_0^s \|\nabla w(\cdot, t)\|^2_{L^2} \, dt = E\left(\phi(\cdot, 0)\right). \tag{1.40}$$

Similarly, the non-conserved gradient equation relative to the energy (1.13), – in other words, the L^2 gradient flow of the energy (1.13) [8] – is expressed as

$$\partial_t \phi = -w, \tag{1.41}$$

which yields the nonlocal Allen-Cahn (nAC) equation (1.3). In this case, classical periodic solutions of Eq. (1.3) (not rigorously defined herein) dissipate the energy E (1.13) at the following rate:

$$d_t E(\phi) = - \|w\|^2_{L^2(\Omega)} \,. \tag{1.42}$$

Weak solutions of Eq. (1.3) (again, not rigorously defined herein) also dissipate the energy E (1.13), but the rate of dissipation is expressed as

$$E\left(\phi(\cdot,s)\right)+\int_0^s \|w(\cdot,t)\|_{L^2}^2\,dt = E\left(\phi(\cdot,0)\right). \tag{1.43}$$

Remark 1.2.3. *The weak energy dissipation rates are important in Chap. 4 and 5. The energy stability proved in these two chapters can be viewed as discrete versions of Eq. (1.40) and Eq. (1.43).*

1.3 Brief Physical Interpretation

So far we have introduced our models only from the mathematical point of view. But in this section we attempt to briefly discuss the physical background of the nCH and nAC equations. Generally speaking, ϕ will represent an indicator function of different states of a physical body that occupies the domain Ω. The function ϕ is often called an *order parameter*. In the material sciences context, ϕ could describe the states of matter or the concentration of one of the constituent species of the material at a point.

For instance, consider a binary crystalline material, that is, a material comprised of species A and species B atoms on a uniform lattice. Suppose that ϕ represents the concentration of species A, where $\phi(\mathbf{x}) = 1$ means that species A occupies all of the possible lattice sites near the point $\mathbf{x}$, that is, species A is at 100% capacity around $\mathbf{x}$. The expression $\phi = -1$ means that no species A is found near $\mathbf{x}$, that is, A is at 0% capacity around $\mathbf{x}$. Suppose ϕ_B gives the same information for species B.

Typically one uses the so-called 'no-gaps' approximation, represented mathematically via $\phi_B = -\phi$. This reflects the simplifying assumption that all lattice sites are occupied at all times, and no atoms are found at interstitial (non-lattice) sites. Thus when A is at 100% capacity at a point, B is at 0% capacity at the point, and *vice versa*. Practically and mathematically, only ϕ is needed to characterize the concentrations of both species in the material. This interpretation of ϕ is the one used in the now classical works of Cahn and Hilliard [11, 9]. We discuss the relationship between the classical (local) Cahn-Hilliard equation and the nCH equation (1.2) momentarily.

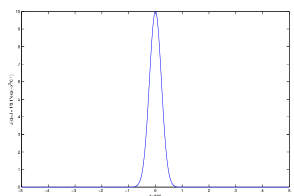
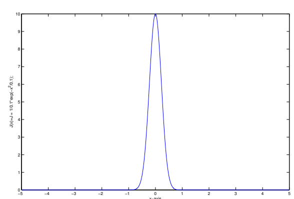
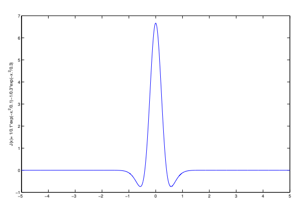
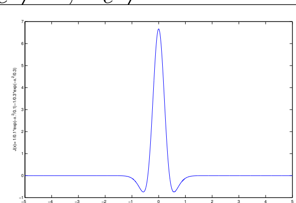
The interpretation of ϕ in the dynamic density functional theory (DDFT) is somewhat different [2, 28, 16]. There ϕ represents something like an atomic probability density, where local relative minima of ϕ may be interpreted as describing the positions the atoms in the material. One can view the nCH equation (1.2) as a version of DDFT equation. The reader is referred to Sec. 1.6 and the references listed therein for more details.

In the case of a binary material, the correlation function J represents the (possibly long range) interactions between atoms at different lattice sites. In the decomposition $J = J_c - J_e$, J_c represents the force of like-like repulsion. In other words, J_c measures the tendency of a pair of type A particles, a given distance apart, to repulse each other. (Equivalently, because of the no-gaps assumption, J_c measures the tendency of A and B particles to attract each other.) Similarly, $-J_e$ represents the force of like-like attraction. Recall both J_c and J_e are non-negative. Of course it is possible (and in fact usual) that J_c and J_e have different spatial profiles. Two particles could be attracted to each other when separated by a distance r_1, and repelled by each other when separated by a distance $r_2 \neq r_1$.

In this paper we use the following notation: if $J_c \not\equiv 0$ and $J_e \equiv 0$, the corresponding nCH and nAC equations are called Repulsive nCH (RnCH) and Repulsive nAC (RnAC) equations; if $J_c \not\equiv 0$ and $J_e \not\equiv 0$ – this is the most general case – the corresponding nCH and nAC equations are called Repulsive-Attractive nCH (RAnCH) and Repulsive-Attractive nAC (RAnAC) equations. See Tab. 1.1. We point out that the RAnCH equation is very closely related to the equation from DDFT [2, 28, 16], though, ϕ does not in that setting have the interpretation as the composition of a binary crystal.

Although the repulsive only and repulsive-attractive cases are both important, the computational results dissertation focus mainly on the more general repulsive-attractive scenario. For the rest of this dissertation the nCH and nAC equations always stand for the more general RAnCH and RAnAC equations, unless specified. All of the theoretical results presented in this dissertation work for both cases.

Table 1.1: The comparison between local and nonlocal equations.

Plot of correlation function J	Corresponding IPDE	Localized approximation
 $J_c \not\equiv 0,\ J_e \equiv 0$	RnCH equation: $\partial_t \phi = \Delta w$.	Classical CH equation [11]: $\partial_t \phi = \Delta \mu$.
 $J_c \not\equiv 0,\ J_e \equiv 0$	RnAC equation: $\partial_t \phi = -w$.	Classical AC equation [10]: $\partial_t \phi = -\mu$.
 $J_c \not\equiv 0,\ J_e \not\equiv 0$	RAnCH equation or DDFT: $\partial_t \phi = \Delta w$.	PFC equation [39]: $\partial_t \phi = \Delta \mu_\star$.
 $J_c \not\equiv 0,\ J_e \not\equiv 0$	RAnAC equation: $\partial_t \phi = -w$.	SH equation [33]: $\partial_t \phi = -\mu_\star$.

1.4 Comparison of Repulsive nCH and Classical Cahn-Hilliard Equation

In this section we discuss the relation between the Repulsive nonlocal Cahn-Hilliard and Allen-Cahn equations with widely used classical Cahn-Hilliard and Allen-Cahn equations. This topic has been discussed intensively, and the reader is directed to [16, 1, 8, 41] and their references for further details. Here we just give a brief discussion. We begin with the Ginzburg-Landau energy

$$G(\phi) = \int_\Omega \left(F(\phi) + \frac{\epsilon^2}{2} |\nabla\phi|^2 \right) d\mathbf{x} \ . \tag{1.44}$$

Again, $\int_\Omega F(\phi) d\mathbf{x}$ is referred to as the homogeneous energy, and $F(\phi)$ is the corresponding homogeneous energy density function. The term $\int_\Omega \frac{\epsilon^2}{2} |\nabla\phi|^2 d\mathbf{x}$ is referred to as the gradient part of the energy. Similar to nCH and nAC we define the chemical potential of classical (local) Cahn-Hilliard and Allen-Cahn equations to be the variational derivative of G:

$$\mu := \delta_\phi G = F'(\phi) - \epsilon^2 \Delta\phi. \tag{1.45}$$

The chemical potential μ can also be divided into two parts: the variational derivative of the homogeneous energy is referred to as the homogeneous part of the chemical potential; the variational derivative of gradient energy is referred to as the gradient part of the chemical potential. The classical (local) Cahn-Hilliard equation is the H^{-1} gradient flow of G [11, 9]:

$$\partial_t \phi = \Delta\mu. \tag{1.46}$$

Here again we use periodic boundary conditions. Similar to the nCH equation, for classical CH equation $\int_\Omega \phi(\mathbf{x}, t) dx = \int_\Omega \phi(\mathbf{x}, 0) dx$. The same energy dissipation rates can be derived: classical periodic solutions of Eq. (1.46) dissipate the energy G (1.44) at the following rate:

$$d_t G(\phi) = -\left\|\nabla\mu\right\|^2_{L^2(\Omega)}. \tag{1.47}$$

Weak solutions of Eq. (1.46) also dissipate the energy G (1.44), but the rate is presented in weak form:

$$G\left(\phi(\cdot,s)\right) + \int_0^s \left\|\nabla\mu(\cdot,t)\right\|^2_{L^2} dt = G\left(\phi(\cdot,0)\right). \tag{1.48}$$

Similarly, the L^2 gradient flow yields the classical (local) Allen-Cahn equation [10]:

$$\partial_t\phi = -\mu. \tag{1.49}$$

Classical periodic solutions of Eq. (1.49) dissipate the energy G (1.44) at the following rate:

$$d_t G(\phi) = -\left\|\mu\right\|^2_{L^2(\Omega)}. \tag{1.50}$$

Weak solutions of Eq. (1.49) also dissipate the energy G (1.44):

$$G\left(\phi(\cdot,s)\right) + \int_0^s \left\|\mu(\cdot,t)\right\|^2_{L^2} dt = G\left(\phi(\cdot,0)\right). \tag{1.51}$$

It is shown in [16, 1, 8, 41] that the energy (1.44) is the approximation of energy (1.13). One way to derive such an approximation is via a Taylor expansion. Specifically, one takes the approximation $(\phi(\mathbf{x})-\phi(\mathbf{y})) \approx (\mathbf{x}-\mathbf{y})\cdot\nabla\phi(\mathbf{x})$ and observes

$$\begin{aligned}\frac{1}{4}\int J(\mathbf{x}-\mathbf{y})\left(\phi(\mathbf{x})-\phi(\mathbf{y})\right)^2 d\mathbf{y} &\approx \frac{1}{4}\int J(\mathbf{x}-\mathbf{y})\left((\mathbf{x}-\mathbf{y})\cdot\nabla\phi(\mathbf{x})\right)^2 d\mathbf{y} \\ &= \frac{\epsilon^2}{2}|\nabla\phi|^2,\end{aligned} \tag{1.52}$$

where $\epsilon^2 = \frac{1}{2}\int_\Omega J(\mathbf{x})|\mathbf{x}|^2\,d\mathbf{x}$ is the second moment of J.

Another way to obtain such a comparison is by looking at the Fourier image of the gradient part of chemical potentials (1.36) and (1.45) used in the nonlocal and classical Cahn-Hilliard and Allen-Cahn equations. For simplicity let us discuss the one-dimensional case, but the results in two-dimensional case can be obtained easily with the same idea. Let us suppose that the function $J = J_c$ ($J_e \equiv 0$) used in the RnCH and RnAC equations is a Gaussian function:

$$J(x) = \frac{1}{\sqrt{\sigma}} e^{-\frac{x^2}{\sigma}}. \tag{1.53}$$

The shape of this potential is shown in Fig. 1.2. For simplicity let us denote $\Omega = (-\infty, \infty)$, and the convolution operator in this specific case is the traditional convolution. Denote by $\widehat{\phi}$ to be the Fourier image of the function ϕ. Since the (nonlinear) homogeneous part in both cases are the same, we simply ignore it in the comparison. Note that the Fourier spectral image of the gradient part used in nonlocal Cahn-Hilliard and Allen-Cahn equations is

$$\widehat{(J*1)\phi} - \widehat{J*\phi} = (J*1)\,\widehat{\phi} - \widehat{J}\,\widehat{\phi}, \tag{1.54}$$

and

$$\widehat{J} = \sqrt{\pi} e^{-\frac{\sigma k^2}{4}}, \quad J*1 = \sqrt{\pi}. \tag{1.55}$$

The Taylor expansion of $J*1-\widehat{J}$ yields

$$J*1-\widehat{J} = \sqrt{\pi} - \sqrt{\pi} + \frac{\sqrt{\pi}\sigma k^2}{4} - \frac{\sqrt{\pi}\sigma^2 k^4}{16} + \cdots \ . \tag{1.56}$$

At the same time Fourier image of gradient part in the potential of classical Cahn-Hilliard and Allen-Cahn equations is

$$\widehat{-\epsilon^2 \Delta \phi} = \epsilon^2 k^2 \widehat{\phi}. \tag{1.57}$$

Note that with the given Gaussian form of J in $\Omega = (-\infty, \infty)$,

$$\epsilon^2 = \frac{1}{2}\int_{-\infty}^{\infty} J(x)|x|^2 dx = \frac{1}{\sqrt{\sigma}}\left[\frac{1}{4}\sigma^{\frac{3}{2}}\sqrt{\pi}\mathrm{erf}\left(\frac{x}{\sqrt{\sigma}}\right) - \frac{1}{2}\sigma x e^{-\frac{x^2}{\sigma}}\right]_{-\infty}^{\infty} = \frac{\sqrt{\pi}\sigma}{4}. \tag{1.58}$$

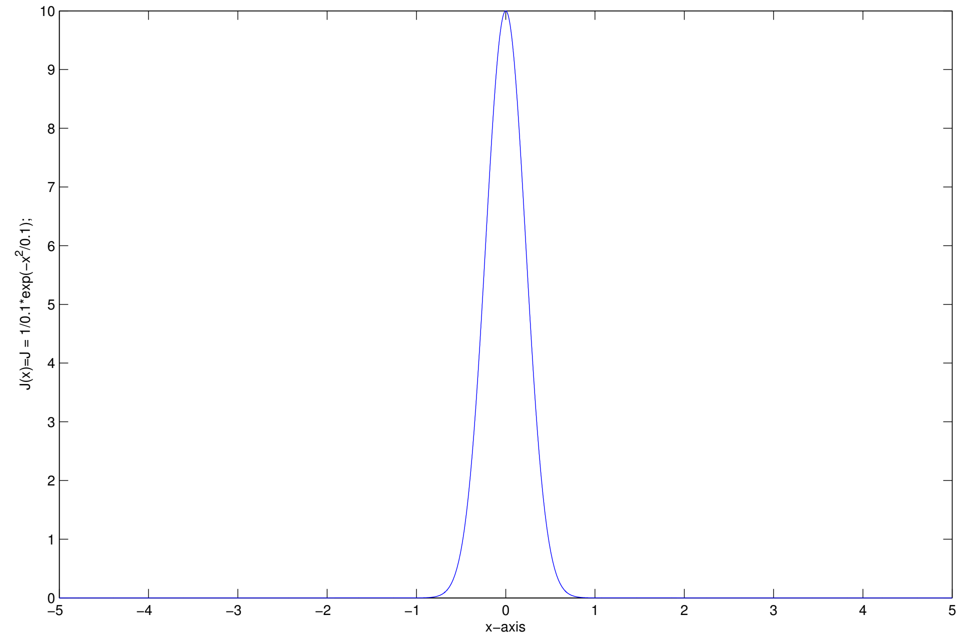


Figure 1.2: The illustration of one-dimensional repulsive potential.

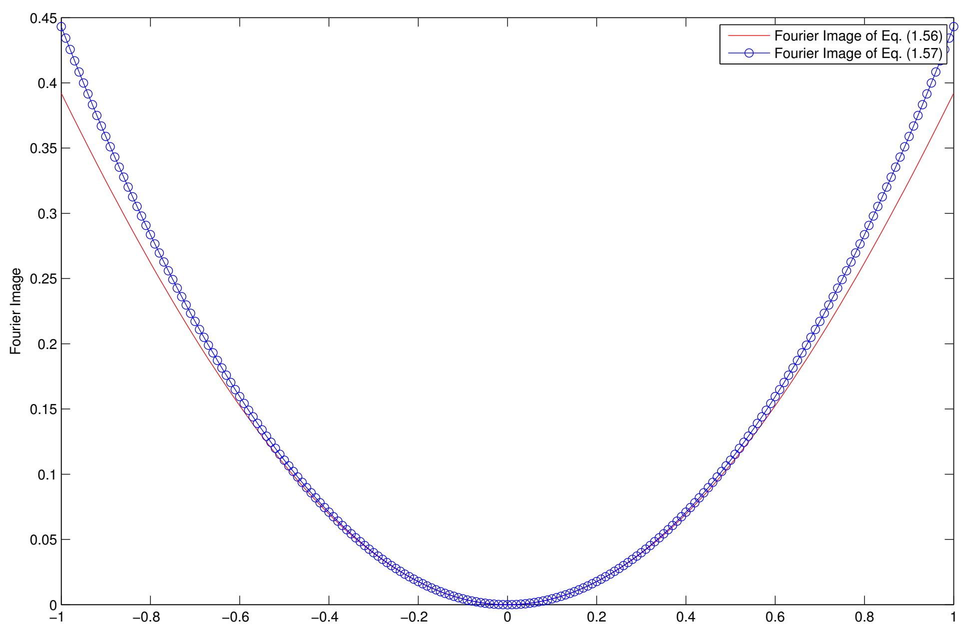


Figure 1.3: The plot of Eq. (1.56) and (1.57).

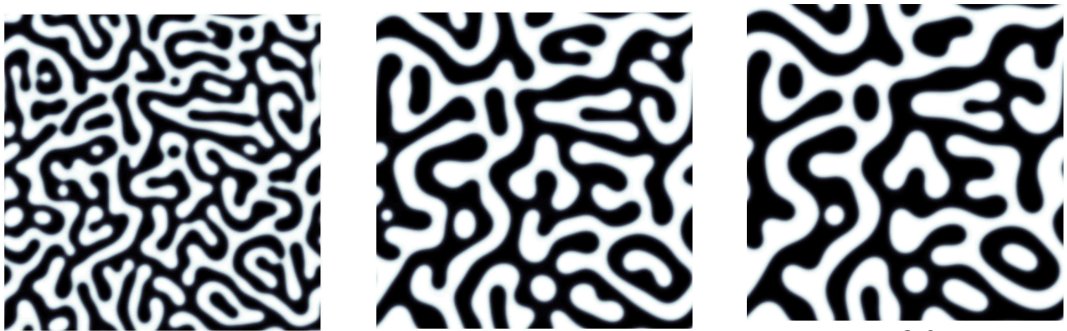


Figure 1.4: Spinodal decomposition as simulated using the nonlocal RnCH equation. Details of this example computation can be found in Chap. 6.

Thus we can see that the local and nonlocal models behave similarly in the Fourier spectrum, as shown in Fig. 1.3. Because of this, solutions of the nonlocal RnCH equation can be used to describe spinodal decomposition, similar to classical CH equation. Figure 1.4 shows the results of a RnCH equation; and the typical spinodal behavior is observed.

1.5 Comparison of Repulsive-Attractive nCH and Phase Field Crystal Equation

In this section we discuss the relationship between the RAnCH equation – which we will, for that sake of brevity, simply identify with the equation from the DDFT – and phase field crystal (PFC) equations. The PFC equation is defined in [39] as

$$\partial_t \phi = \Delta \mu_\star \ , \tag{1.59}$$

where

$$\mu_\star := \phi^3 + (\gamma_c - \gamma_e)\phi + 2\Delta\phi - \Delta^2\phi \ . \tag{1.60}$$

$\mu_\star$ is referred as the chemical potential of PFC equation, the homogeneous part and gradient part of $\mu_\star$ is defined in the same fashion as for w (1.36) and μ (1.45).

Similarly, the Swift-Hohenberg (SH) equation is defined in [33] as

$$\partial_t \phi = -\mu_\star \ . \tag{1.61}$$

The PFC equation is an attempt in approximating the DDFT equation through differential operators. Observe that the (local) PFC equation is fundamentally different that the (local) classical CH equation. For instance the second-order differential operator in the chemical potential $\mu_\star$ is negative, or backward diffusive. The fourth-order term, of course, regularizes the situation so that the PFC equation is well-posed. Again, the PFC and SH equations dissipate an energy. See [39] and references therein for more details.

We are going to apply the same idea and setting in previous section. However, in this case we consider the correlation function

$$J(x) = \frac{\alpha}{\sqrt{\sigma_1}} e^{-\frac{x^2}{\sigma_1}} - \frac{\beta}{\sqrt{\sigma_2}} e^{-\frac{x^2}{\sigma_2}}, \tag{1.62}$$

where α, β, σ_1 and σ_2 are positive constants. In this case J is capable of modeling both repulsion and attraction. See Fig. 1.6. The Fourier image of the operator in the gradient part of w now becomes:

$$J*1-\widehat{J} = (\alpha-\beta)\sqrt{\pi}-(\alpha-\beta)\sqrt{\pi}+\frac{\sqrt{\pi}\alpha\sigma_1 k^2}{4}-\frac{\sqrt{\pi}\beta\sigma_2 k^2}{4}-\frac{\sqrt{\pi}\alpha\sigma_1^2 k^4}{16}+\frac{\sqrt{\pi}\beta\sigma_2^2 k^4}{16}+\cdots \ . \tag{1.63}$$

On the other hand, the Fourier image of the operator in the gradient part of $\mu_\star$ now becomes:

$$2\widehat{\Delta\phi} - \widehat{\Delta^2\phi} = (-2k^2 + k^4)\widehat{\phi}. \tag{1.64}$$

Naturally, with certain choices of the parameters α, β and σ_1, σ_2, a Fourier image comparison can be made, similar to what was done for the comparison between the

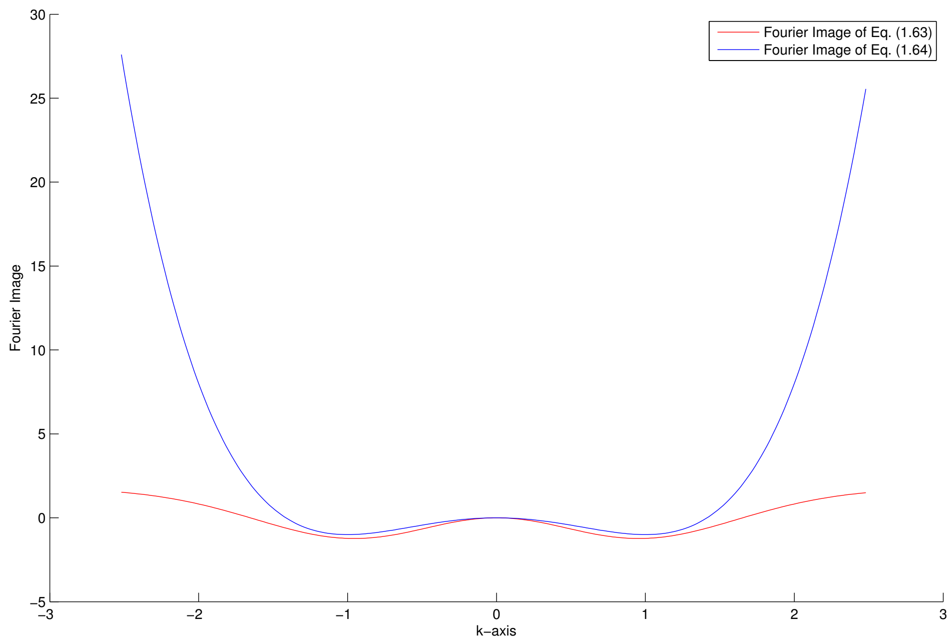


Figure 1.5: The comparison between RAnCH and PFC equations in Fourier spectrum

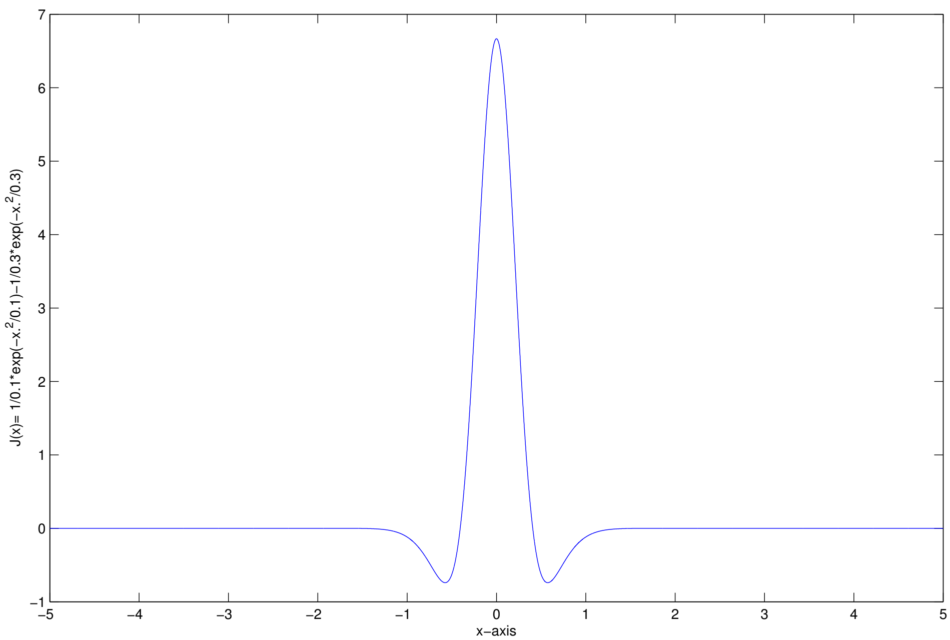


Figure 1.6: The illustration of a one-dimensional repulsive-attractive correlation function J.

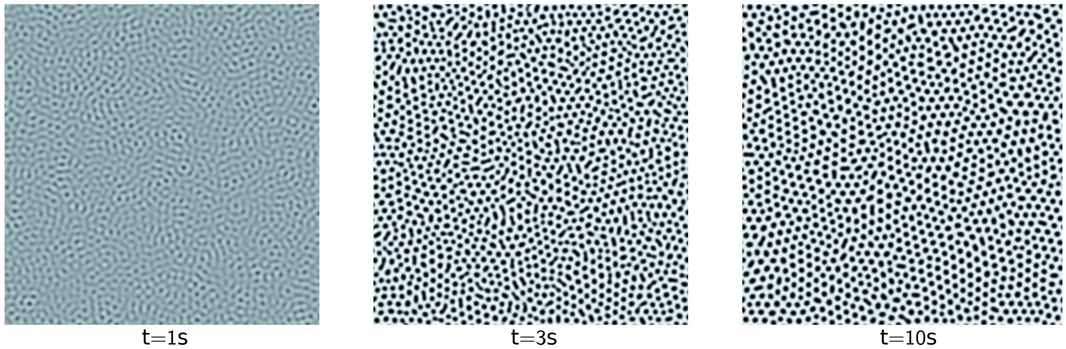


Figure 1.7: A simulation of RAnCH equation (with repulsive-attractive correlation function J). The details of this example computation can be found in Chap. 6. Note the formation of nearly regularly space local minima of ϕ (black dots). These dots can be interpreted as the atoms of a crystallizing solid, or as the aggregates in a colloidal mixture.

RnCH and Classical CH equations in the previous section. See Fig. 1.5. And this finding hints that RAnCH is capable of simulating crystallization phenomena, as shown in Fig. 1.7. In a similar way, the comparison between RAnAC and SH equations can be made.

Remark 1.5.1. *To summarize the comparisons we made in Secs. 1.4 and1.5, it is clear that nCH and nAC can mimic many different widely-used equations. Everything depends upon the choice of the correlation function J. See, for example, Tab. 1.1.*

1.6 Previous Works

The nonlocal Cahn-Hilliard type energy can be understood as a special form of the Helmholtz free energy functional, which is derived from studying the interaction of particles. Nowadays this concept is widely used in many areas such as statistical physics, material sciences, continuum thermodynamics, bio-mathematics and fluid dynamics. The derivation of Helmholtz free energy functional is an extensively studied topic and reader is referred to [41, 26, 32, 20] for more details.

The construction of the Helmholtz free energy functional in the dynamical density functional theory (DDFT) is quite a complicated undertaking. We refer readers to [16, 28, 2] for details. We also refer readers to [3] for the detailed discussion of the construction of correlation function. Recently it has become quite common to approximate the equation of motion from the DDFT by truncating the nonlocal operators in Fourier space (as we have shown) by a polynomial in the wave number k. Essentially the nonlocal operator is replaced by partial derivatives. This is the main idea of the phase field crystal (PFC) methodology. See, for example, [39, 34, 13] and references therein for more about the PFC modeling framework. DDFT is successfully used in the study of to crystal growth in single and binary materials [14, 27, 35], and many other fields in physics and material sciences which share the same dynamics, for instance, the implication of DDFT in tumor growth [41, 42, 12].

Although the application of DDFT is extensive, the study of the nonlinear, nonlocal models Eq. (1.2) and Eq. (1.3) is rather recent. There are only a few results concerning the integro-differential equation analysis. See [20, 21, 19, 6, 7, 4] and references therein for nCH. See [4, 8, 17] and references therein for nAC. See [29, 31, 30] and references therein for other aspects of nonlocal interaction models.

There are also some previous results regarding to the numerical simulation of Eq. (1.2) and Eq. (1.3). In [24] the spectral method was applied in solving nonlocal Cahn-Hilliard type problem. In [18] an efficient scheme was developed for nonlocal Cahn-Hilliard with specific boundary condition. In [5] a mixed finite difference scheme for nonlocal Allen-Cahn was developed and the property of propagation is discussed. In [23] the spectral method was applied in solving nonlocal Allen-Cahn type problem with stochastic terms. However to the best of authors' knowledge this paper is the first second order in time scheme for those problems. The convergence of the numerical simulation of (1.3) is also the first result so far.

1.7 Contribution of This Dissertation Work

The following represent our primary contributions in this dissertation.

1. We propose and analyze a family of two-dimensional unconditionally energy stable schemes for these IPDEs (Chap. 4 and 5). Specifically, we prove following properties of these schemes:

   - These schemes are uniquely solvable, independent of time and space step sizes (Sec. 4.5 and Sec. 5.4).
   - These schemes are energy stable, independent of time and space step sizes (Sec. 4.6 and Sec. 5.5).
   - These schemes are convergent, provided the time step sizes are sufficiently small (Sec. 4.7 and Sec. 5.6).

2. We develop a highly efficient solver for schemes we propose. These schemes are semi-implicit and contain nonlinear implicit terms, which makes numerical solutions challenging. To overcome this difficulty, a nearly-optimally efficient nonlinear multigrid method is employed (Sec. 6.2).

3. Via our numerical methods, we are able to simulate crystal nucleation and growth phenomena, with arbitrary crystalline anisotropy, with properly chosen parameters for nonlocal Cahn-Hilliard equation, in a very efficient and straightforward way (Sec. 6.5).

Also there are some important supplementary results we'd like to address:

- We prove some inequalities which is very efficient in estimating discrete inner product with nonlinear terms and convolution terms without L^∞ bounds (Chap. 2 and 3).
- We provide the numerical evidence that there schemes converge with the expected order (Sec. 6.3 and Sec. 6.4).

To our best knowledge, no similar results has been achieved in this field.

Chapter 2

The One-Dimensional Discrete Space: Basic Tools and Important Estimates

2.1 Overview

Our primary goal in this chapter is to define the discretized one-dimensional space together discrete operators and prove some crucial inequalities which will be used as the motivation of inequalities in Chap. 3.

There are already many useful results regarding to the norms, discrete difference operators and summation-by-parts formulas from works by C. Wang, S.M. Wise and J.S. Lowengrub [38, 40, 39]. Thus we are going to follow the setting established in [40, 39].

However, due to the special property of the IPDEs like nCH and nAC, the existing results are not enough to provide the foundation of numerical analysis. Therefore we define the discrete convolution operator on discrete one-dimensional space and discuss its properties. Also there is a problem obtaining the L^∞ bound for solutions in those schemes. Thus we prove some inequalities in this chapter as well. They will play an important in the proof of the convergence of schemes.

Although our main results in this paper is in two-dimensional discrete space, we still want to present the result in one-dimensional space. The first reason is that with results provided in this chapter, the proof of similar schemes for nCH and nAC equations in one-dimensional space is straightforward. The second reason is that the proof of their two-dimensional counter parts use essentially the same method, thus one-dimensional version serves as the motivation.

The chapter will be organized in the following way: Sec. 2.2 defines the discrete one-dimensional space with difference operators borrowing the notation and results from [40, 39], the summation-by-parts formulas will also be presented; Sec. 2.3 defines the one-dimensional discrete periodic convolution operator with discussion of its properties; Sec. 2.4 presents the proof for some identities which will be important later; Sec. 2.5 defines a family of cut-off functions and an important estimate regarding to them.

2.2 The Discretization of One-Dimensional Space

Here we use the notation and results from [40, 39]. We begin with definitions of grid functions and difference operators needed for our discretization of one-dimensional space. For simplicity suppose $\Omega = (0, L)$, Let $h = L/n$, where $n \in \mathbb{Z}^+$. We define the function $p_r = p(r) := (r - \frac{1}{2}) \cdot h$, where r takes on integer and half-integer values, and the following three sets $E_n = \{p_{i+\frac{1}{2}} \mid i = 0, \ldots, n\}$, $C_n = \{p_i \mid i = 1, \ldots, n\}$, and $C_{\overline{n}} = \{p_i \mid i = 0, \ldots, n+1\}$. We define by $\mathcal{E}_n$ the space of functions whose domains equal E_n. The functions of $\mathcal{E}_n$ are called edge-centered functions, and we reserve the symbols f and g to denote them. In component form, these functions are identified via $f_{i+\frac{1}{2}} := f(p_{i+\frac{1}{2}})$ for $i = 0, \ldots, n$. By $\mathcal{C}_n$ we denote the vector space of functions whose domains are equal to C_n, and by $\mathcal{C}_{\overline{n}}$ we denote the space of functions whose domains equal to $C_{\overline{n}}$. The functions of $\mathcal{C}_n$ and $\mathcal{C}_{\overline{n}}$ are called cell centered functions,

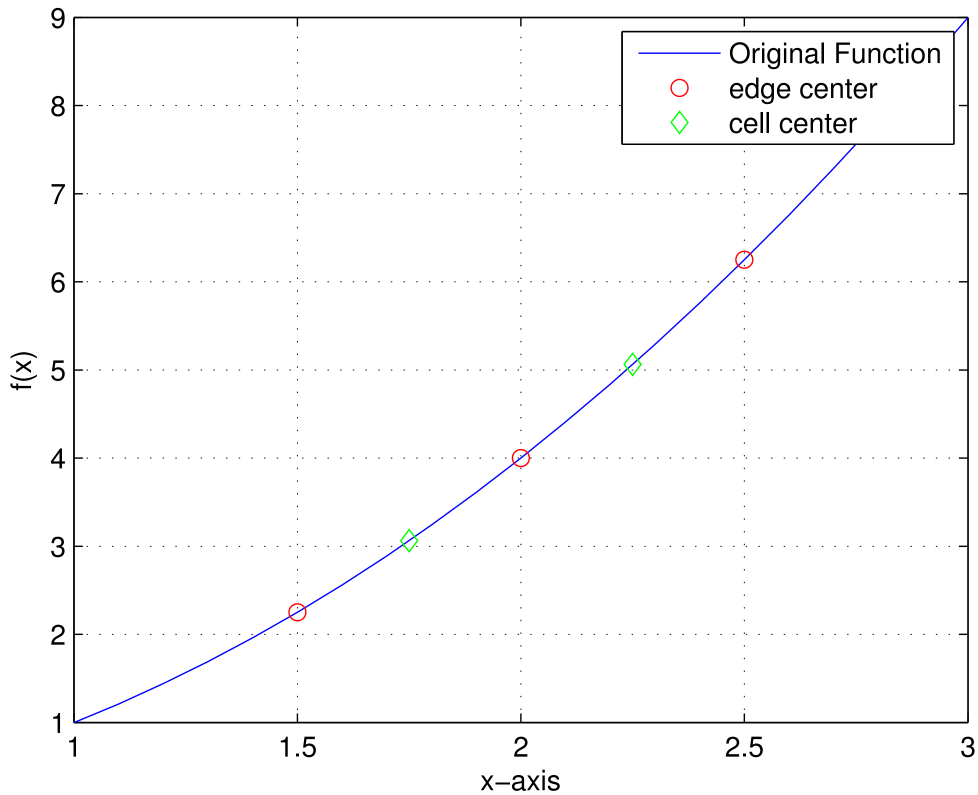


Figure 2.1: The illustration of one-dimensional cell and edge centered discretization. The size of the mesh is 0.5.

and we use the Greek symbols ϕ, ψ, and ζ to denote them. In component form, these functions are identified via $\phi_i := \phi(p_i)$, where $i = 1, \dots, n$, if $\phi \in \mathcal{C}_n$, and $i = 0, \dots, n+1$, if $\phi \in \mathcal{C}_{\overline{n}}$.

Let ϕ and ψ be cell-centered, and let f and g be edge-centered. Fig. 2.1 is an example of the position for those functions on one-dimensional mesh. We define the respective inner products on $\mathcal{C}_n$ and $\mathcal{E}_n$

$$(\phi|\psi) = \sum_{i=1}^{n} \phi_i \psi_i, \quad [f|g] = \frac{1}{2} \sum_{i=1}^{n} \left(f_{i-\frac{1}{2}} g_{i-\frac{1}{2}} + f_{i+\frac{1}{2}} g_{i+\frac{1}{2}} \right). \tag{2.1}$$

The edge-to-center difference operator $d : \mathcal{E}_n \to \mathcal{C}_n$, the center-to-edge average and difference operators, respectively, A, $D : \mathcal{C}_{\overline{n}} \to \mathcal{E}_n$, and the discrete Laplacian operator $\Delta_h : \mathcal{C}_{\overline{n}} \to \mathcal{C}_n$ are defined component-wise as

$$df_i = \frac{1}{h}\left(f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}\right),\ i = 1, \ldots, n, \tag{2.2}$$

$$A\phi_{i+\frac{1}{2}} = \frac{1}{2}\left(\phi_i + \phi_{i+1}\right),\ D\phi_{i+\frac{1}{2}} = \frac{1}{h}\left(\phi_{i+1} - \phi_i\right),\ i = 0, \ldots, n, \tag{2.3}$$

$$\Delta_h \phi_i = d\left(D\phi\right)_i = \frac{1}{h^2}\left(\phi_{i-1} - 2\phi_i + \phi_{i+1}\right),\ i = 1, \ldots, n. \tag{2.4}$$

We shall say the cell-centered function $\phi \in \mathcal{C}_m$ is periodic if and only if, for all $p \in \mathbb{Z}^+$,

$$\phi_{i+p\cdot m} = \phi_i \quad i = 1, \ldots, m. \tag{2.5}$$

Notice that ϕ is not explicitly defined on an infinite grid. But ϕ can be extended as a periodic function in a perfectly natural way, which is the context in which we view the last definition. Similar definitions are available for periodic edge and vertex centered grid functions.

The following summation-by-parts formulas are borrowed from [39]:

Proposition 2.2.1. *Let ϕ, $\psi \in \mathcal{C}_{\overline{n}}$ and $f \in \mathcal{E}_n$. Then*

$$h\ [D\phi|f] = -h\ (\phi|df) - A\phi_{\frac{1}{2}} f_{\frac{1}{2}} + A\phi_{n+\frac{1}{2}} f_{n+\frac{1}{2}}, \tag{2.6}$$

$$h\ [D\phi|D\psi] = -h\ (\phi|\Delta_h\psi) - A\phi_{\frac{1}{2}} D\psi_{\frac{1}{2}} + A\phi_{n+\frac{1}{2}} D\psi_{n+\frac{1}{2}}, \tag{2.7}$$

$$\begin{aligned} h\ (\phi|\Delta_h\psi) = {} & h\ (\Delta_h\phi|\psi) + A\phi_{n+\frac{1}{2}} D\psi_{n+\frac{1}{2}} - D\phi_{n+\frac{1}{2}} A\psi_{n+\frac{1}{2}} \\ & - A\phi_{\frac{1}{2}} D\psi_{\frac{1}{2}} + D\phi_{\frac{1}{2}} A\psi_{\frac{1}{2}}. \end{aligned} \tag{2.8}$$

With the definition of periodic function Prop. (2.2.1) can be simplified further straightforwardly.

Proposition 2.2.2. *Let ϕ, $\psi \in \mathcal{C}_n$ and $f \in \mathcal{E}_n$, ϕ, ψ and f are periodic. Then*

$$h\,[D\phi|f] = -h\,(\phi|df)\,, \tag{2.9}$$

$$h\,[D\phi|D\psi] = -h\,(\phi|\Delta_h\psi)\,, \tag{2.10}$$

$$h\,(\phi|\Delta_h\psi) = h\,(\Delta_h\phi|\psi)\,. \tag{2.11}$$

We also borrow the definition of norms from [39] for cell-centered functions. If $\phi \in \mathcal{C}_m$, then $\|\phi\|_2 := \sqrt{h\,(\phi\|\phi)}$, $\|\phi\|_4 := \sqrt{h\,(\phi^4\|\mathbf{1})}$, and $\|\phi\|_\infty := \max_{1\le i\le m}|\phi_i|$. We define $\|\nabla_h\phi\|_2$, where $\phi \in \mathcal{C}_m$ and periodic, to mean

$$\|D\phi\|_2 := \sqrt{h\,[D\phi|D\phi]}\,. \tag{2.12}$$

2.3 Discrete Periodic Convolution Operator

Here we define the one-dimensional discrete periodic convolution operator. If $\phi \in \mathcal{C}_n$, $\varphi \in \mathcal{E}_n$, ϕ and φ are periodic, then the discrete convolution operator $[\varphi \star \phi] : \mathcal{E}_n \times \mathcal{C}_n \to \mathcal{C}_n$ is defined component-wise as:

$$[\varphi \star \phi]_i = h\sum_{k=1}^{n}\varphi_{k+\frac{1}{2}}\phi_{i-k} = h\sum_{k=1}^{n}\varphi_{i-k+\frac{1}{2}}\phi_k. \tag{2.13}$$

We can prove following properties for $[\cdot \star \cdot]$:

Lemma 2.3.1. *If $\phi, \psi \in \mathcal{C}_n$ are periodic, $\varphi \in \mathcal{E}_n$ is even and periodic, then*

$$(\phi|[\varphi \star \psi]) = (\psi|[\varphi \star \phi])\ . \tag{2.14}$$

Proof. By definition

$$(\phi|[\varphi \star \psi]) = h\sum_{i=1}^{n}\phi_i\sum_{k=1}^{n}\varphi_{i-k+\frac{1}{2}}\psi_k\ . \tag{2.15}$$

Since φ is an even function, for any i,k

$$\varphi_{i-k+\frac{1}{2}} = \varphi\left((i-k)\cdot h\right) = \varphi\left((k-i)\cdot h\right) = \varphi_{k-i+\frac{1}{2}}.$$

Thus

$$\begin{aligned} h\sum_{i=1}^{n}\phi_i\sum_{k=1}^{n}\varphi_{i-k+\frac{1}{2}}\psi_k =& h\sum_{i=1}^{n}\sum_{k=1}^{n}\phi_i\varphi_{k-i+\frac{1}{2}}\psi_k \\ =& h\sum_{k=1}^{n}\psi_k\sum_{i=1}^{n}\varphi_{k-i+\frac{1}{2}}\phi_i \ . \end{aligned}$$

By definition,

$$h\sum_{k=1}^{n}\psi_k\sum_{i=1}^{n}\varphi_{k-i+\frac{1}{2}}\phi_i = (\psi|[\varphi\star\phi]) \ .$$

□

Lemma 2.3.2. *If $\phi, \psi \in \mathcal{C}_n$ are periodic and $\varphi \in \mathcal{E}_n$ is even, positive and periodic, then, for any $\alpha > 0$,*

$$|\,(\phi|[\varphi\star\psi])\,| \leq \frac{\alpha}{2}\,[\varphi\star 1]\,(\phi|\phi) + \frac{1}{2\alpha}\,[\varphi\star 1]\,(\psi|\psi) \ . \tag{2.16}$$

If $f, g \in \mathcal{E}_n$ are periodic and $\varphi \in \mathcal{E}_n$ is even, positive and periodic, then, for any $\alpha > 0$,

$$|\,[f|[\varphi\star g]\,]\,| \leq \frac{\alpha}{2}\,[\varphi\star 1]\,[f|f] + \frac{1}{2\alpha}\,[\varphi\star 1]\,[g|g] \ . \tag{2.17}$$

Proof. The definition shows that

$$
\begin{aligned}
|\left(\phi|[\varphi\star\psi]\right)| \leq & h\sum_{i=1}^{n}\sum_{k=1}^{n}\varphi_{k+\frac{1}{2}}|\phi_{i-k}\psi_i| \\
\leq & h\sum_{i=1}^{n}\sum_{k=1}^{n}\varphi_{k+\frac{1}{2}}\frac{1}{2}\left(\phi_{i-k}^2+\psi_i^2\right) \\
\leq & \frac{\alpha}{2}\left(1\middle|\left[\varphi\star\phi^2\right]\right)+\frac{1}{2\alpha}\left[\varphi\star 1\right](\psi|\psi) \\
= & \frac{\alpha}{2}\left(\phi^2\middle|[\varphi\star 1]\right)+\frac{1}{2\alpha}\left[\varphi\star 1\right](\psi|\psi) \\
= & \frac{\alpha}{2}\left[\varphi\star 1\right](\phi|\phi)+\frac{1}{2\alpha}\left[\varphi\star 1\right](\psi|\psi)\ .
\end{aligned}
$$

In a similar way, the case for edge function can also be proved.

□

Lemma 2.3.3. *If $\phi\in\mathcal{C}_n$ is periodic, $J\in C^\infty\Omega$ is even, periodic, and $J_{i+\frac{1}{2}}:=J(x_{i+\frac{1}{2}})$. Then*

$$
-2h\left(\left[J\star\phi\right]|\Delta_h\phi\right)\leq M_{10}\frac{1}{\alpha_2}\left\|\phi\right\|_2^2+\alpha_2\left\|D\phi\right\|_2^2\ . \tag{2.18}
$$

Proof. Using summation-by-parts

$$
\begin{aligned}
-2h\left(\left[J\star\phi\right]|\Delta_h\left(\phi\right)\right)= & 2h\left[D\left[J\star\phi\right]|D\phi\right] \\
\leq & \frac{h}{\alpha_2}\left[\left(D\left[J\star\phi\right]\right)^2\middle|1\right]+\alpha_2 h\left[1\middle|(D\phi)^2\right]\ .
\end{aligned} \tag{2.19}
$$

By the definition of discrete operator, we have

$$
\begin{aligned}
D\left[J\star\phi\right]_{i+\frac{1}{2}}= & \frac{1}{h}\left(h\sum_{k=1}^{n}J_{(i+1)-k+\frac{1}{2}}\phi_k-h\sum_{k=1}^{n}J_{i-k+\frac{1}{2}}\phi_k\right) \\
= & h\sum_{k=1}^{n}\frac{1}{h}\left(J_{(i+1)-k+\frac{1}{2}}-J_{i-k+\frac{1}{2}}\right)\phi_k \\
= & h\sum_{k=1}^{n}\left(dJ_{i-k}\right)\phi_k\ .
\end{aligned} \tag{2.20}
$$

By the definition of J there exists a constant C independent of h, such that $\|dJ\|_\infty < C$. Therefore

$$D\left[J \star \phi\right]_{i+\frac{1}{2}} \leq Ch \sum_{k=1}^{n} \phi_k. \tag{2.21}$$

Thus by discrete Hölder inequality

$$\left(D\left[J \star \phi\right]_{i+\frac{1}{2}}\right)^2 \leq C^2 h^2 \left(\sum_{k=1}^{n} \phi_k\right)^2 \leq C^2 h^2 n \sum_{k=1}^{n} \phi_k^2 = C^2 |\Omega| \left\|\phi\right\|_2^2 \ . \tag{2.22}$$

Therefore

$$\frac{h}{\alpha_2} \left[\left(D\left[J \star \phi\right]\right)^2 \middle| 1 \right] \leq \frac{C^2 |\Omega|^2}{\alpha_2} \left\|\phi\right\|_2^2 \ . \tag{2.23}$$

The result follows immediately. □

2.4 General Identities and Inequalities

In this section we present some one-dimensional discrete identities which will be used in the convergence proof for the first and second schemes for nCH and nAC.

Lemma 2.4.1. *If $\phi, \psi \in \mathcal{C}_n$ are periodic, $(\phi - \psi | 1) = 0$ and $\|\phi\|_4 < C_1, \|\psi\|_4 < C_2$, and $\|\phi\|_\infty < C_3, \|D\phi\|_\infty < C_4$, where C_1, C_2, C_3 and C_4 are positive constants independent of h, then there exists a positive constant M_1 independent of h, such that*

$$2h\left(\phi^3 - \psi^3 \middle| \Delta_h\left(\phi - \psi\right)\right) \leq M_1 \left\|D\left(\phi - \psi\right)\right\|_2^2 \ . \tag{2.24}$$

Proof. Using summation-by-parts,

$$2h\left(\phi^3 - \psi^3 \middle| \Delta_h\left(\phi - \psi\right)\right) = -2h\left[D\left(\phi^3 - \psi^3\right) \middle| D\left(\phi - \psi\right)\right] \ .$$

Denote

$$\mathbb{A}\phi_{i+\frac{1}{2}} = \frac{1}{2}\phi_{i+1}^2 + \frac{1}{2}\phi_i^2 + \frac{1}{2}\left(\phi_{i+1}+\phi_i\right)^2 \ . \tag{2.25}$$

By definition

$$D\phi^3_{i+\frac{1}{2}} = \frac{1}{h}\left(\phi_{i+1}^3 - \phi_i^3\right) = \left[\phi_{i+1}^2 + \phi_i^2 + \phi_{i+1}\phi_i\right] D\phi_{i+\frac{1}{2}} = \mathbb{A}\phi_{i+\frac{1}{2}} D\phi_{i+\frac{1}{2}} \ , \tag{2.26}$$

$$D\psi^3_{i+\frac{1}{2}} = \frac{1}{h}\left(\psi_{i+1}^3 - \psi_i^3\right) = \left[\psi_{i+1}^2 + \psi_i^2 + \psi_{i+1}\psi_i\right] D\psi_{i+\frac{1}{2}} = \mathbb{A}\psi_{i+\frac{1}{2}} D\psi_{i+\frac{1}{2}} \ . \tag{2.27}$$

Thus

$$-2h\left[D\left(\phi^3-\psi^3\right)\middle| D\left(\phi-\psi\right)\right] = -2h\left[\mathbb{A}\phi D\phi - \mathbb{A}\psi D\psi | D\left(\phi-\psi\right)\right] \ .$$

By adding and subtracting $\mathbb{A}\psi D\phi$, we have

$$\begin{aligned} &-2h\left[D\left(\phi^3-\psi^3\right)\middle| D\left(\phi-\psi\right)\right] \\ =&-2h\left[\mathbb{A}\phi D\phi + \mathbb{A}\psi D\phi - \mathbb{A}\psi D\phi - \mathbb{A}\psi D\psi | D\left(\phi-\psi\right)\right] \ . \end{aligned}$$

Noticing that

$$\left[\mathbb{A}\psi D\phi - \mathbb{A}\psi D\psi | D\left(\phi-\psi\right)\right] = \left[\mathbb{A}\psi\middle|\left(D\left(\phi-\psi\right)\right)^2\right] \ .$$

This together with $\mathbb{A}\psi \geq 0$ yields

$$\begin{aligned} -2h\left[D\left(\phi^3-\psi^3\right)\middle| D\left(\phi-\psi\right)\right] \leq& -2h\left[\mathbb{A}\phi D\phi - \mathbb{A}\psi D\phi | D\left(\phi-\psi\right)\right] \\ \leq& 2h\left|\left[\mathbb{A}\phi D\phi - \mathbb{A}\psi D\phi | D\left(\phi-\psi\right)\right]\right| \\ \leq& 2h\left[\left(|\mathbb{A}\phi - \mathbb{A}\psi|\right)\left(|D\phi|\right)|\left(|D\left(\phi-\psi\right)|\right)\right] \ . \end{aligned}$$

Since $\|\phi\|_\infty < C_3, \|D\phi\|_\infty < C_4$,

$$-2h\left[D\left(\phi^3-\psi^3\right)\middle| D\left(\phi-\psi\right)\right] \leq 2hC_4\left[\left(|\mathbb{A}\phi - \mathbb{A}\psi|\right)|\left(|D\left(\phi-\psi\right)|\right)\right] \ .$$

By Hölder inequality, we obtain

$$2h\left[(|\mathbb{A}\phi-\mathbb{A}\psi|)|(|D\left(\phi-\psi\right)|)\right] \leq 2h\left[\left(\mathbb{A}\phi-\mathbb{A}\psi\right)^2\Big|1\right]^{\frac{1}{2}}\left[\left(D\left(\phi-\psi\right)\right)^2\Big|1\right]^{\frac{1}{2}} \ .$$

Also noticing that

$$\begin{aligned}
\left(\mathbb{A}\phi-\mathbb{A}\psi\right)_{i+\frac{1}{2}} =& \frac{1}{2}\left(\phi_{i+1}\right)^2+\frac{1}{2}\left(\phi_i\right)^2+\frac{1}{2}\left(\phi_{i+1}+\phi_i\right)^2 \\
&-\frac{1}{2}\left(\psi_{i+1}\right)^2-\frac{1}{2}\left(\psi_i\right)^2-\frac{1}{2}\left(\psi_{i+1}+\psi_i\right)^2 \\
=&\frac{1}{2}\left(\phi_{i+1}+\psi_{i+1}\right)\left(\phi_{i+1}-\psi_{i+1}\right)+\frac{1}{2}\left(\phi_i+\psi_i\right)\left(\phi_i-\psi_i\right) \\
&+\frac{1}{2}\left(\phi_{i+1}+\psi_{i+1}+\phi_i+\psi_i\right)\left(\phi_{i+1}-\psi_{i+1}+\phi_i-\psi_i\right) \ .
\end{aligned}$$

Thus

$$\begin{aligned}
\left(\mathbb{A}\phi-\mathbb{A}\psi\right)^2_{i+\frac{1}{2}} \leq& \frac{3}{4}\left(\phi_{i+1}+\psi_{i+1}\right)^2\left(\phi_{i+1}-\psi_{i+1}\right)^2+\frac{3}{4}\left(\phi_i+\psi_i\right)^2\left(\phi_i-\psi_i\right)^2 \\
&+\frac{3}{4}\left(\phi_{i+1}+\psi_{i+1}+\phi_i+\psi_i\right)^2\left(\phi_{i+1}-\psi_{i+1}+\phi_i-\psi_i\right)^2 \\
\leq& \frac{3}{4}\left(\phi_{i+1}+\psi_{i+1}\right)^2\left(\phi_{i+1}-\psi_{i+1}\right)^2+\frac{3}{4}\left(\phi_i+\psi_i\right)^2\left(\phi_i-\psi_i\right)^2 \\
&+3\left(\left(\phi_{i+1}+\psi_{i+1}\right)^2+\left(\phi_i+\psi_i\right)^2\right)\left(\left(\phi_{i+1}-\psi_{i+1}\right)^2+\left(\phi_i-\psi_i\right)^2\right) \\
\leq& \frac{15}{4}\left(\left(\phi_{i+1}+\psi_{i+1}\right)^2+\left(\phi_i+\psi_i\right)^2\right)\left(\left(\phi_{i+1}-\psi_{i+1}\right)^2+\left(\phi_i-\psi_i\right)^2\right) \ .
\end{aligned} \tag{2.28}$$

Similarly,

$$\left(\mathbb{A}\phi-\mathbb{A}\psi\right)^2_{i-\frac{1}{2}} \leq \frac{15}{4}\left(\left(\phi_{i-1}+\psi_{i-1}\right)^2+\left(\phi_i+\psi_i\right)^2\right)\left(\left(\phi_{i-1}-\psi_{i-1}\right)^2+\left(\phi_i-\psi_i\right)^2\right) \ . \tag{2.29}$$

Denote

$$\mathbb{H}_{i+\frac{1}{2}} = \frac{1}{2}\left((\phi_{i+1}+\psi_{i+1})^2 + (\phi_i+\psi_i)^2\right) \ , \tag{2.30}$$

$$\mathbb{G}_{i+\frac{1}{2}} = \frac{1}{2}\left((\phi_{i+1}-\psi_{i+1})^2 + (\phi_i-\psi_i)^2\right) \ . \tag{2.31}$$

By the definition of $[\cdot|\cdot]$ and Hölder inequality, we see that

$$\begin{aligned}\left[(\mathbb{A}\phi - \mathbb{A}\psi)^2\middle|1\right] &\leq 15\,[\mathbb{H}|\mathbb{G}] \\ &\leq 15\left[\mathbb{H}^2\middle|1\right]^{\frac{1}{2}}\left[1\middle|\mathbb{G}^2\right]^{\frac{1}{2}} \ .\end{aligned} \tag{2.32}$$

The definition of $\mathbb{H}_{i+\frac{1}{2}}$ shows that

$$\begin{aligned}\mathbb{H}^2_{i+\frac{1}{2}} &= \frac{1}{4}\left((\phi_{i+1}+\psi_{i+1})^2 + (\phi_i+\psi_i)^2\right)^2 \\ &\leq 4\left((\phi_{i+1})^4 + (\psi_{i+1})^4 + (\phi_i)^4 + (\psi_i)^4\right) \ .\end{aligned} \tag{2.33}$$

Thus by the definition of $[\cdot|\cdot]$ and the periodic condition, we get

$$\left[\mathbb{H}^2\middle|1\right] \leq \frac{8}{h}\left\|\phi\right\|_4^4 + \frac{8}{h}\left\|\psi\right\|_4^4 \ . \tag{2.34}$$

Similarly,

$$\left[1\middle|\mathbb{G}^2\right] \leq \frac{1}{h}\left\|\phi-\psi\right\|_4^4 \ . \tag{2.35}$$

Thus

$$\left[(\mathbb{A}\phi - \mathbb{A}\psi)^2\middle|1\right] \leq \frac{1}{h}\left[1800\left(\left\|\phi\right\|_4^4 + \left\|\psi\right\|_4^4\right)\right]^{\frac{1}{2}}\left\|\phi-\psi\right\|_4^2 \ . \tag{2.36}$$

Also

$$\left[\left(D\left(\phi-\psi\right)\right)^2\middle|1\right]^{\frac{1}{2}} = \frac{1}{\sqrt{h}}\left\|D\left(\phi-\psi\right)\right\|_2 \ . \tag{2.37}$$

Combining the above results,

$$-2h\left[D\left(\phi^3-\psi^3\right)\middle|D\left(\phi-\psi\right)\right] \le 2C_4\left[1800\left(\|\phi\|_4^4+\|\psi\|_4^4\right)\right]^{\frac{1}{4}}\|\phi-\psi\|_4\|D\left(\phi-\psi\right)\|_2 \ . \tag{2.38}$$

We borrowed a lemma proved from [38] which yields that under the condition $(\phi-\psi|1)=0$,

$$\|\phi-\psi\|_4 \le C_5\|D\left(\phi-\psi\right)\|_2 \ , \tag{2.39}$$

where C_5 is a constant independent of h. Therefore

$$2h\left(\phi^3-\psi^3\middle|\Delta_h\left(\phi-\psi\right)\right) \le 2\left[1800\left(\|\phi\|_4^4+\|\psi\|_4^4\right)\right]^{\frac{1}{4}}C_4C_5\|D\left(\phi-\psi\right)\|_2^2 \ . \tag{2.40}$$

By the assumption of $\|\phi\|_4$ and $\|\psi\|_4$, the result follows. □

2.5 Cut-off Functions and Their Properties

In this section we are going to define a family of cut-off function and propose an important estimate involving them.

Proposition 2.5.1. *There exists a cut-off function $F_{M_3}(u) \in C^3(\mathbb{R})$ for positive constant M_3 defined as:*

$$F_{M_3}(u) = \begin{cases} u^3, & \left|\frac{u}{M_3}\right| \in [0,1) \\ \epsilon_1(u), & \frac{u}{M_3} \in [1,2) \\ C_1u+M_3^1, & \frac{u}{M_3} \in [2,+\infty) \\ \epsilon_2(u), & \frac{u}{M_3} \in (-2,-1] \\ C_2u-M_3^2, & \frac{u}{M_3} \in (+\infty,-2] \end{cases} \tag{2.41}$$

where the function ϵ_1 and ϵ_2 satisfies:

1) $\epsilon_1(u) \in C^\infty[1,2)$ and $\epsilon_2(u) \in C^\infty(-2,-1]$.

2) $\epsilon_1(M_3) = (M_3)^3$, $\epsilon_1'(M_3) = 3\,(M_3)^2$, $\epsilon_1''(M_3) = 6M_3$.

3) $\lim_{u\to 2M_3^-} \epsilon_1(u) = 2C_1M_3 + M_3^1$*, where* $2C_1M_3 + M_3^1 > (M_3)^3$.

4) $\lim_{u\to 2M_3^-} \epsilon_1'(u) = C_1$, $\lim_{u\to 2M_3^-} \epsilon_1''(u) = 0$.

5) $\epsilon_2(-M_3) = (-M_3)^3$, $\epsilon_2'(-M_3) = 3\,(-M_3)^2$, $\epsilon_2''(-M_3) = -6M_3$.

6) $\lim_{u\to -2M_3^+} \epsilon_2(u) = -C_2M_3 - 2M_3^2$*, where* $-2C_2M_3 - M_3^2 < (-M_3)^3$.

7) $\lim_{u\to -2M_3^+} \epsilon_2'(u) = C_2$, $\lim_{u\to -2M_3^+} \epsilon_2''(u) = 0$.

8) ϵ_1 *and* ϵ_2 *are increasing.*

This implies

$$F'_{M_3}(u) = \begin{cases} 3u^2, & \left|\frac{u}{M_3}\right| \in [0,1) \\ \epsilon_1'(u), & \frac{u}{M_3} \in [1,2) \\ C_1, & \frac{u}{M_3} \in [2,+\infty) \\ \epsilon_2'(u), & \frac{u}{M_3} \in (-2,-1] \\ C_2, & \frac{u}{M_3} \in (+\infty,-2] \end{cases} \tag{2.42}$$

and

$$F''_{M_3}(u) = \begin{cases} 6u. & \left|\frac{u}{M_3}\right| \in [0,1) \\ \epsilon_1''(u). & \frac{u}{M_3} \in [1,2) \\ \epsilon_2''(u). & \frac{u}{M_3} \in (-2,-1] \\ 0. & else \end{cases} \tag{2.43}$$

Remark 2.5.1. *Although presented in this chapter, Prop. 2.5.1 is actually independent of dimension of u. Therefore it can also be applied into two-dimensional space of higher.*

Lemma 2.5.1. *If* $\phi, \psi \in \mathcal{C}_n$ *are periodic,* $\|\phi\|_\infty < C_3$, $\|D\phi\|_\infty < \infty < C_4$*, where* C_3, C_4 *are positive constants independent of* h*. Let* $M_3 > 0$ *be given and* F_{M_3} *is defined as Prop. 2.5.1, then*

$$2h\left(F_{M_3}(\phi) - F_{M_3}(\psi) | \Delta_h(\phi-\psi)\right) \le \frac{M_4}{\alpha_1}\|\phi-\psi\|_2^2 + \alpha_1 M_5 \|D(\phi-\psi)\|_2^2 + \frac{M_6}{\alpha_1}h^4\ , \tag{2.44}$$

where M_4, M_5 and M_6 are positive constants independent of h, but depend on M_3.

Proof. Using summation-by-parts, we have

$$2h\left(F_{M_3}(\phi) - F_{M_3}(\psi)|\Delta_h(\phi-\psi)\right) = -2h\left[D\left(F_{M_3}(\phi) - F_{M_3}(\phi)\right)|D(\phi-\psi)\right] \ .$$

Denote

$$\delta_h F_{M_3}(\phi)_{i+\frac{1}{2}} = \frac{\left[F_{M_3}(\phi_{i+1}) - F_{M_3}(\phi_i)\right]}{\left[\phi_{i+1}-\phi_i\right]}, \quad \delta_h F_{M_3}(\psi)_{i+\frac{1}{2}} = \frac{\left[F_{M_3}(\psi_{i+1}) - F_{M_3}(\psi_i)\right]}{\left[\psi_{i+1}-\psi_i\right]}. \tag{2.45}$$

Since F_{M_3} is increasing, $\delta_h F_{M_3}(\phi) \geq 0$, $\delta_h F_{M_3}(\psi) \geq 0$. An application of Taylor expansion shows that

$$F_{M_3}(\phi_{i+1}) - F_{M_3}(\phi_i) = F'_{M_3}(\phi_i)(\phi_{i+1}-\phi_i) + \frac{1}{2}F''_{M_3}(\xi_i)(\phi_{i+1}-\phi_i)^2 \tag{2.46}$$

where $\xi_i \in [\phi_i, \phi_{i+1}]$. By definition,

$$\begin{aligned} DF_{M_3}(\phi)_{i+\frac{1}{2}} =& \frac{1}{h}\left[F_{M_3}(\phi_{i+1}) - F_{M_3}(\phi_i)\right] = \frac{\left[F_{M_3}(\phi_{i+1}) - F_{M_3}(\phi_i)\right]}{\left[\phi_{i+1}-\phi_i\right]}\frac{\left[\phi_{i+1}-\phi_i\right]}{h} \\ =& \delta_h F_{M_3}(\phi)_{i+\frac{1}{2}} D\phi_{i+\frac{1}{2}} \ . \end{aligned} \tag{2.47}$$

Similarly,

$$DF_{M_3}(\psi)_{i+\frac{1}{2}} = \delta_h F_{M_3}(\psi)_{i+\frac{1}{2}} D\psi_{i+\frac{1}{2}} \ . \tag{2.48}$$

Thus

$$\begin{aligned} & -2h\left[D\left(F_{M_3}(\phi) - F_{M_3}(\psi)\right)|D(\phi-\psi)\right] \\ =& -2h\left[\delta_h F_{M_3}(\phi) D\phi - \delta_h F_{M_3}(\psi) D\psi | D(\phi-\psi)\right] \ . \end{aligned} \tag{2.49}$$

By adding and subtracting $\delta_h F_{M_3}(\psi) D\phi$,

$$
\begin{aligned}
& -2h\left[D\left(F_{M_3}(\phi)-F_{M_3}(\psi)\right)|D(\phi-\psi)\right] \\
= & -2h\left[\delta_h F_{M_3}(\phi) D\phi-\delta_h F_{M_3}(\psi) D\phi|D(\phi-\psi)\right] \\
& -2h\left[\delta_h F_{M_3}(\psi) D\phi-\delta_h F_{M_3}(\psi) D\psi|D(\phi-\psi)\right] .
\end{aligned}
$$

Notice that

$$
-2h\left[\delta_h F_{M_3}(\psi) D\phi-\delta_h F_{M_3}(\psi) D\psi|D(\phi-\psi)\right]=-2h\left[\delta_h F_{M_3}(\psi)\Big|(D(\phi-\psi))^2\right] . \tag{2.50}
$$

This together with $\delta_h F_{M_3}(\psi) \geq 0$ yields

$$
\begin{aligned}
& -2h\left[D\left(F_{M_3}(\phi)-F_{M_3}(\psi)\right)|D(\phi-\psi)\right] \\
\leq & -2h\left[\left(\delta_h F_{M_3}(\phi)-\delta_h F_{M_3}(\psi)\right) D\phi|D(\phi-\psi)\right] \\
\leq & 2h\left|\left[\left(\delta_h F_{M_3}(\phi)-\delta_h F_{M_3}(\psi)\right) D\phi|D(\phi-\psi)\right]\right| \\
\leq & 2h\left[\left(\left|\delta_h F_{M_3}(\phi)-\delta_h F_{M_3}(\psi)\right|\right)(|D\phi|)|\left(\left|D_x(\phi-\psi)\right|\right)\right] .
\end{aligned} \tag{2.51}
$$

By the fact that $\|\phi\|_\infty < C_3$, $\|D\phi\|_\infty < C_4$, we get

$$
\begin{aligned}
& -2h\left[D\left(F_{M_3}(\phi)-F_{M_3}(\psi)\right)|D(\phi-\psi)\right] \\
\leq & 2hC_4\left[\left(\left|\delta_h F_{M_3}(\phi)-\delta_h F_{M_3}(\psi)\right|\right)|(|D(\phi-\psi)|)\right] .
\end{aligned} \tag{2.52}
$$

By the Taylor expansion,

$$
\begin{aligned}
&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2}} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2}}\right| \\
=&\left|\frac{F'_{M_3}(\phi_i)(\phi_{i+1}-\phi_i) + \frac{1}{2}F''_{M_3}(\xi_i)(\phi_{i+1}-\phi_i)^2}{\phi_{i+1}-\phi_i}\right. \\
&\left. - \frac{F'_{M_3}(\psi_i)(\psi_{i+1}-\psi_i) + \frac{1}{2}F''_{M_3}(\eta_i)(\psi_{i+1}-\psi_i)^2}{\psi_{i+1}-\psi_i}\right| \\
\leq&\left|F'_{M_3}(\phi_i) - F'_{M_3}(\psi_i)\right| + \frac{1}{2}\left|F''_{M_3}(\xi_i)(\phi_{i+1}-\phi_i) - F''_{M_3}(\eta_i)(\psi_{i+1}-\psi_i)\right|.
\end{aligned} \tag{2.53}
$$

By Prop. 2.5.1, it is easy to prove F'_{M_3} is Lipschitz continuous. Thus

$$
\begin{aligned}
&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2}} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2}}\right| \\
\leq& 6M_3\left|\phi_i - \psi_i\right| + \frac{1}{2}\left|F''_{M_3}(\xi_i)(\phi_{i+1}-\phi_i) - F''_{M_3}(\eta_i)(\psi_{i+1}-\psi_i)\right|.
\end{aligned} \tag{2.54}
$$

Notice that

$$
\begin{aligned}
&\left|F''_{M_3}(\xi_i)(\phi_{i+1}-\phi_i) - F''_{M_3}(\eta_i)(\psi_{i+1}-\psi_i)\right| \\
=&\left|F''_{M_3}(\xi_i)\phi_{i+1} - F''_{M_3}(\xi_i)\phi_i - F''_{M_3}(\eta_i)\psi_{i+1} + F''_{M_3}(\eta_i)\psi_i\right|.
\end{aligned} \tag{2.55}
$$

Adding and subtracting $F''_{M_3}(\eta_i)\phi_{i+1}$ and $F''_{M_3}(\xi_i)\psi_i$ gives

$$
\begin{aligned}
&\left|F''_{M_3}(\xi_i)(\phi_{i+1}-\phi_i) - F''_{M_3}(\eta_i)(\psi_{i+1}-\psi_i)\right| \\
=&\left|\left[F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right]\phi_{i+1} + F''_{M_3}(\eta_i)\left[\phi_{i+1}-\psi_{i+1}\right]\right. \\
&\left. - \left[F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right]\psi_i - F''_{M_3}(\xi_i)\left[\phi_i-\psi_i\right]\right| \\
\leq&\left|F''_{M_3}(\eta_i)\left[\phi_{i+1}-\psi_{i+1}\right]\right| + \left|F''_{M_3}(\xi_i)\left[\phi_i-\psi_i\right]\right| \\
&+\left|\left[F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right]\right|\left|\phi_{i+1}-\psi_i\right|.
\end{aligned} \tag{2.56}
$$

By the property of F''_{M_3}, $F''_{M_3} \leq 12M_3$,

$$
\begin{aligned}
&\left| F''_{M_3}(\xi_i)(\phi_{i+1}-\phi_i) - F''_{M_3}(\eta_i)(\psi_{i+1}-\psi_i) \right| \\
\leq &12M_3\left|\phi_{i+1}-\psi_{i+1}\right| + 12M_3\left|\phi_i-\psi_i\right| + \left|\left[F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right]\right|\left|\phi_{i+1}-\psi_i\right| . \qquad (2.57)
\end{aligned}
$$

Furthermore, adding and subtracting ϕ_i yields

$$
\begin{aligned}
&\left|\left[F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right]\right|\left|\phi_{i+1}-\psi_i\right| \\
=&\left|\left[F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right]\right|\left|\phi_{i+1}-\phi_i+\phi_i-\psi_i\right| \\
\leq&\left|F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right|\left|\phi_{i+1}-\phi_i\right| + \left|F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right|\left|\phi_i-\psi_i\right| \\
\leq&\left|F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right|\left|\phi_{i+1}-\phi_i\right| + 24M_3\left|\phi_i-\psi_i\right| . \qquad (2.58)
\end{aligned}
$$

By multiplying and dividing h, $\phi_{i+1} - \phi_i = hD\phi_{i+\frac{1}{2}}$, together with the Lipschitz continuity of F''_{M_3}, we have

$$
\left|F''_{M_3}(\xi_i) - F''_{M_3}(\eta_i)\right|\left|\phi_{i+1}-\phi_i\right| \leq 6M_3hC_4\left|\xi_i-\eta_i\right| . \qquad (2.59)
$$

By the definition of ξ_i and η_i,

$$
\begin{aligned}
\left|\xi_i-\eta_i\right| \leq&\left|\phi_{i+1}-\psi_{i+1}\right| + \left|\phi_i-\psi_i\right| + \left|\phi_{i+1}-\psi_i\right| + \left|\phi_i-\psi_{i+1}\right| \\
\leq&\left|\phi_{i+1}-\psi_{i+1}\right| + \left|\phi_i-\psi_i\right| + \left|\phi_{i+1}-\phi_i\right| \\
&+\left|\phi_i-\psi_i\right| + \left|\phi_i-\phi_{i+1}\right| + \left|\phi_{i+1}-\psi_{i+1}\right| \\
\leq&2\left|\phi_{i+1}-\psi_{i+1}\right| + 2\left|\phi_i-\psi_i\right| + 2hC_4 . \qquad (2.60)
\end{aligned}
$$

Combining the above results,

$$
\begin{aligned}
&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2}} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2}}\right| \\
\leq & 6M_3|\phi_i - \psi_i| + 6M_3|\phi_{i+1} - \psi_{i+1}| + 6M_3|\phi_i - \psi_i| + 12M_3|\phi_i - \psi_i| \\
&+ 6M_3 h C_4 \left(|\phi_{i+1} - \psi_{i+1}| + |\phi_i - \psi_i| + hC_4\right) \ . \qquad (2.61)
\end{aligned}
$$

Without lose of generality, we can assume that h is small. Thus

$$
\begin{aligned}
&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2}} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2}}\right| \\
\leq & 48M_3 \left(\frac{1}{2}|\phi_{i+1} - \psi_{i+1}| + \frac{1}{2}|\phi_i - \psi_i|\right) + 6M_3 \|D\phi\|_\infty^2 h^2 \\
= & 48M_3 \left(A|\phi - \psi|_{i+\frac{1}{2}}\right) + 6M_3 C_4^2 h^2 \ . \qquad (2.62)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&-2h\left[D\left(F_{M_3}(\phi) - F_{M_3}(\phi)\right) | D(\phi - \psi)\right] \\
\leq & 2hC_4 \left[48M_3 \left(A|\phi - \psi|\right) + 6M_3 C_4^2 h^2 \middle| \left(|D(\phi - \psi)|\right)\right] \ . \qquad (2.63)
\end{aligned}
$$

By Cauchy inequality and the definition of $[\cdot|\cdot]$, we arrive at

$$
\begin{aligned}
&-2h\left[D\left(F_{M_3}(\phi) - F_{M_3}(\phi)\right) | D(\phi - \psi)\right] \\
\leq & 2hC_4 \frac{4}{\alpha_1} (48M_3)^2 \left[\left(A|\phi - \psi|\right)^2 \middle| 1\right] + 2hC_4 \frac{4}{\alpha_1} \left(6M_3 C_4^2\right)^2 \left[h^4 \middle| 1\right] \\
&+ 2hC_4 \frac{\alpha_1}{2} \left[1 \middle| \left(D(\phi - \psi)\right)^2\right] \\
\leq & 2C_4 \frac{4}{\alpha_1} (48M_3)^2 \|\phi - \psi\|_2^2 + 2C_4 \frac{\alpha_1}{2} \|D(\phi - \psi)\|_2^2 + 2C_4 \frac{4}{\alpha_1} \left(6M_3 C_4^2\right)^2 |\Omega| h^4. \qquad (2.64)
\end{aligned}
$$

Thus the proof follows. □

Chapter 3

The Two-Dimensional Discrete Space: Basic Tools and Important Estimates

3.1 Overview

Our primary goal in this chapter is to define the discretized two-dimensional space together discrete operators and prove some crucial inequalities which will be used in Chap. 4 and 5.

Like the previous chapter we are going to develop our results from [38, 40, 39]. The two-dimensional version of identities and inequalities presented in Sec. 2.4 will be proved.

The chapter will be organized in the following way: Sec. 3.2 defines the discrete two-dimensional space with difference operators borrowing the notation and results from [40, 39], the summation-by-parts formulas will also be presented; Sec. 3.3 defines the two-dimensional discrete periodic convolution operator with discussion of its properties; Sec. 3.4 presents the proof for some identities which serve as lemmas for the error estimates of schemes; Sec. 3.5 presents the estimate involving the cut-off function.

3.2 Discretization of Two-Dimensional Space

In this section we are going to extend the discretization from one-dimensional space to two-dimensional space. For simplicity, let us assume that $\Omega = (0, L_{x_1}) \times (0, L_{x_2})$. Here we use the notation and results for cell-centered functions from [40, 39]. We begin with definitions of grid functions and difference operators needed for our discretization of two-dimensional space. Let $\Omega = (0, L_{x_1}) \times (0, L_{x_2})$, with $L_{x_1} = m \cdot h$ and $L_{x_2} = n \cdot h$, where m and n are positive integers and $h > 0$ is the spatial step size. Define $p_r := (r - \frac{1}{2}) \cdot h$, where r takes on integer and half-integer values. For any positive integer ℓ, define $E_\ell = \left\{ p_r \mid r = \frac{1}{2}, \ldots, \ell + \frac{1}{2} \right\}$, $C_\ell = \{p_r \mid r = 1, \ldots, \ell\}$, $C_{\overline{\ell}} = \{p_r \cdot h \mid r = 0, \ldots, \ell + 1\}$. Define the function spaces

$$\mathcal{C}_{m\times n} = \{\phi : C_m \times C_n \to \mathbb{R}\}, \ \mathcal{C}_{\overline{m}\times\overline{n}} = \{\phi : C_{\overline{m}} \times C_{\overline{n}} \to \mathbb{R}\} \ , \tag{3.1}$$

$$\mathcal{E}^{\rm ew}_{m\times n} = \{u : E_m \times C_n \to \mathbb{R}\}, \ \mathcal{E}^{\rm ns}_{m\times n} = \{v : C_m \times E_n \to \mathbb{R}\} \ , \tag{3.2}$$

$$\mathcal{E}^{\rm ew}_{m\times\overline{n}} = \{u : E_m \times C_{\overline{n}} \to \mathbb{R}\}, \ \mathcal{E}^{\rm ns}_{\overline{m}\times n} = \{v : C_{\overline{m}} \times E_n \to \mathbb{R}\} \ , \tag{3.3}$$

$$\mathcal{V}_{m\times n} = \{f : E_m \times E_n \to \mathbb{R}\} \ . \tag{3.4}$$

We use the notation $\phi_{i,j} := \phi(p_i, p_j)$ for *cell-centered* functions, those in the spaces $\mathcal{C}_{m\times n}$ or $\mathcal{C}_{\overline{m}\times\overline{n}}$. In component form *east-west edge-centered* functions, those in the spaces $\mathcal{E}^{\rm ew}_{m\times n}$ or $\mathcal{E}^{\rm ew}_{m\times\overline{n}}$, are identified via $u_{i+\frac{1}{2},j} := u(p_{i+\frac{1}{2}}, p_j)$. In component form *north-south edge-centered* functions, those in the spaces $\mathcal{E}^{\rm ns}_{m\times n}$, or $\mathcal{E}^{\rm ns}_{\overline{m}\times n}$, are identified via $u_{i+\frac{1}{2},j} := u(p_{i+\frac{1}{2}}, p_j)$. The functions of $\mathcal{V}_{m\times n}$ are called *vertex-centered* functions. In component form vertex-centered functions are identified via $f_{i+\frac{1}{2},j+\frac{1}{2}} := f(p_{i+\frac{1}{2}}, p_{j+\frac{1}{2}})$. Fig. 3.1 is an example of the position for those functions on two-dimensional mesh. We will need the weighted 2D grid inner-products $(\,\cdot\,\|\,\cdot\,)$, $[\,\cdot\,\|\,\cdot\,]_{\rm ew}$,

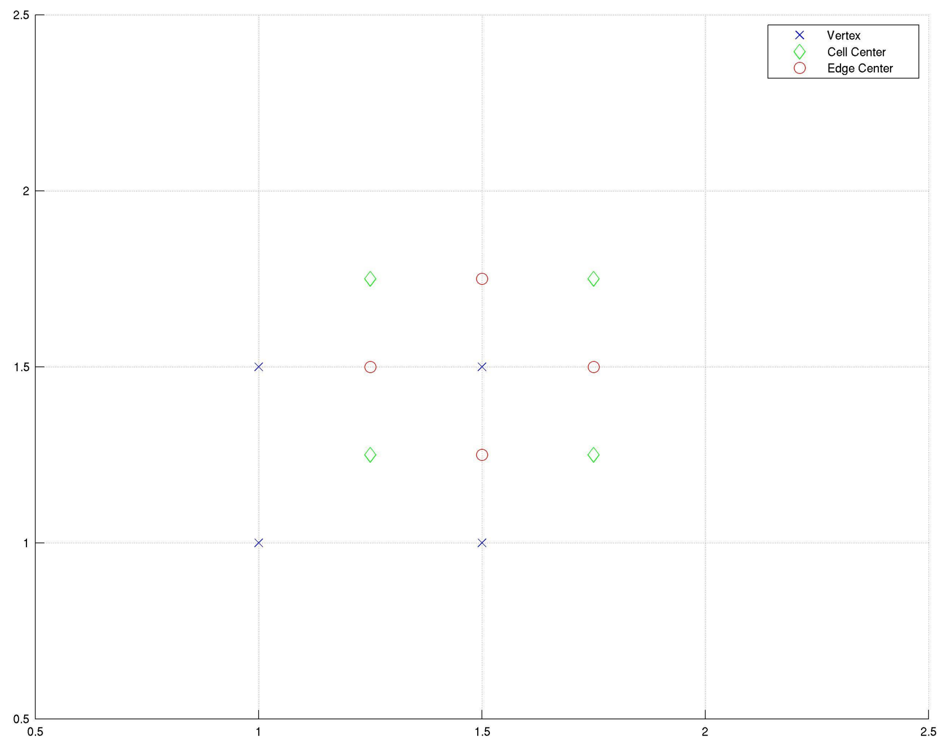


Figure 3.1: The illustration of two-dimensional cell, edge and vertex centered discretization. The size of the mesh is 0.5×0.5.

$[\cdot\|\cdot]_{\text{ns}}$ that are defined in [40, 39]:

$$
\begin{aligned}
(\phi\|\psi) &= \sum_{i=1}^{m}\sum_{j=1}^{n}\phi_{i,j}\psi_{i,j}, \quad \phi,\,\psi\in\mathcal{C}_{m\times n}\cup\mathcal{C}_{\overline{m}\times n}\cup\mathcal{C}_{m\times\overline{n}}\cup\mathcal{C}_{\overline{m}\times\overline{n}}, &(3.5)\\
[f\|g]_{\text{ew}} &= \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{n}\left(f_{i+\frac12,j}g_{i+\frac12,j}+f_{i-\frac12,j}g_{i-\frac12,j}\right), \quad f,\,g\in\mathcal{E}^{\text{ew}}_{m\times n}, &(3.6)\\
[f\|g]_{\text{ns}} &= \frac{1}{2}\sum_{i=1}^{m}\sum_{j=1}^{n}\left(f_{i,j+\frac12}g_{i,j+\frac12}+f_{i,j-\frac12}g_{i,j-\frac12}\right), \quad f,\,g\in\mathcal{E}^{\text{ns}}_{m\times n}. &(3.7)
\end{aligned}
$$

In addition to these, we will use the 2D grid inner product

$$
\begin{aligned}
\langle f\|g\rangle &= \frac{1}{4}\sum_{i=1}^{m}\sum_{j=1}^{n}\big(f_{i+\frac12,j+\frac12}g_{i+\frac12,j+\frac12}+f_{i+\frac12,j-\frac12}g_{i+\frac12,j-\frac12}\\
&\quad +f_{i-\frac12,j+\frac12}g_{i-\frac12,j+\frac12}+f_{i-\frac12,j-\frac12}g_{i-\frac12,j-\frac12}\big), \quad f,\,g\in\mathcal{V}^{\text{ns}}_{m\times n}. &(3.8)
\end{aligned}
$$

The following definition of discrete difference operators is also borrowed from [40, 39]. The edge-to-center differences, $d_x:\mathcal{E}^{\text{ew}}_{m\times n}\to\mathcal{C}_{m\times n}$ and $d_y:\mathcal{E}^{\text{ns}}_{m\times n}\to\mathcal{C}_{m\times n}$; the center-to-edge averages and differences, $A_x, D_x:\mathcal{C}_{\overline{m}\times n}\to\mathcal{E}^{\text{ew}}_{m\times n}$ and $A_y, D_y:\mathcal{C}_{m\times\overline{n}}\to\mathcal{E}^{\text{ew}}_{m\times n}$; and the 2D discrete Laplacian, $\Delta_h:\mathcal{C}_{\overline{m}\times\overline{n}}\to\mathcal{C}_{m\times n}$ are defined component-wise via

$$
\begin{aligned}
d_xf_{i,j} &= \frac{1}{h}\left(f_{i+\frac12,j}-f_{i-\frac12,j}\right),\ d_yf_{i,j}=\frac{1}{h}\left(f_{i,j+\frac12}-f_{i,j-\frac12}\right),\ {\scriptstyle i=1,\ldots,m \atop j=1,\ldots,n}, &(3.9)\\
A_x\phi_{i+\frac12,j} &= \frac{1}{2}\left(\phi_{i,j}+\phi_{i+1,j}\right),\ D_x\phi_{i+\frac12,j}=\frac{1}{h}\left(\phi_{i+1,j}-\phi_{i,j}\right),\ {\scriptstyle i=0,\ldots,m \atop j=1,\ldots,n}, &(3.10)\\
A_y\phi_{i,j+\frac12} &= \frac{1}{2}\left(\phi_{i,j}+\phi_{i,j+1}\right),\ D_y\phi_{i,j+\frac12}=\frac{1}{h}\left(\phi_{i,j+1}-\phi_{i,j}\right),\ {\scriptstyle i=1,\ldots,m \atop j=0,\ldots,n}, &(3.11)\\
\Delta_h\psi_{i,j} &= d_x(D_x\psi)_{i,j}+d_y(D_y\psi)_{i,j},\ {\scriptstyle i=1,\ldots,m \atop j=1,\ldots,n}. &(3.12)
\end{aligned}
$$

Like the one-dimensional case in Sec. 2.2, we shall say the cell-centered function $\phi\in\mathcal{C}_{m\times n}$ is periodic if and only if, for all p, $q\in\mathbb{Z}$,

$$
\phi_{i+p\cdot m,j+q\cdot n}=\phi_{i,j}\quad i=1,\ldots,m,\quad j=1,\ldots,n. \tag{3.13}
$$

Also ϕ is not explicitly defined on an infinite grid. but ϕ can be extended as a periodic function in a perfectly natural way, and we view the last definition just the same way as one-dimensional case. Similar definitions are available for periodic edge and vertex centered grid functions.

We will use the grid function norms defined in [40, 39]. If $\phi \in \mathcal{C}_{m\times n}$, then $\|\phi\|_2 := \sqrt{h^2 (\phi\|\phi)}$, $\|\phi\|_4 := \sqrt{h^2 (\phi^4\|\mathbf{1})}$, and $\|\phi\|_\infty := \max_{\substack{1\le i\le m\\ 1\le j\le n}} |\phi_{i,j}|$. We define $\|\nabla_h\phi\|_2$, where $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$, to mean

$$\|\nabla_h\phi\|_2 := \sqrt{h^2 \left[D_x\phi\|D_x\phi\right]_{\rm ew} + h^2 \left[D_y\phi\|D_y\phi\right]_{\rm ns}} \,. \tag{3.14}$$

We will use the following discrete Sobolev-type norms for grid functions $\phi \in \mathcal{C}_{\overline{m}\times\overline{n}}$: $\|\phi\|_{0,2} := \|\phi\|_2$ and

$$\|\phi\|_{1,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2}, \ \|\phi\|_{2,2} := \sqrt{\|\phi\|_2^2 + \|\nabla_h\phi\|_2^2 + \|\Delta_h\phi\|_2^2} \,. \tag{3.15}$$

We will specifically use the following inverse inequality: for any $\phi \in \mathcal{C}_{m\times n}$ and all $1 \le p < \infty$

$$\|\phi\|_\infty \le h^{-\frac{2}{p}} \|\phi\|_p \,. \tag{3.16}$$

Using the definitions given in this section and in [40, 39], we obtain the following summation-by-parts formulas whose proofs are simple:

Proposition 3.2.1. (summation-by-parts:) *If $\phi \in \mathcal{C}_{m\times n}$ is periodic and $f \in \mathcal{E}^{\rm ew}_{m\times n}$ is periodic then*

$$h^2 \left[D_x\phi\|f\right]_{\rm ew} = -h^2 \left(\phi\|d_x f\right), \tag{3.17}$$

and if $\phi \in \mathcal{C}_{m\times n}$ is periodic and $f \in \mathcal{E}^{\rm ns}_{m\times n}$ is periodic then

$$h^2 \left[D_y\phi\|f\right]_{\rm ns} = -h^2 \left(\phi\|d_y f\right). \tag{3.18}$$

If $f \in \mathcal{V}_{m\times n}$ *is periodic and* $g \in \mathcal{E}^{\rm ns}_{\overline{m}\times n}$ *is periodic then*

$$h^2 \cdot [d_x f \| g]_{\rm ns} = -h^2 \cdot \langle f \| D_x g \rangle \,, \tag{3.19}$$

and if $f \in \mathcal{V}_{m\times n}$ *is periodic and* $g \in \mathcal{E}^{\rm ew}_{m\times\overline{n}}$ *is periodic then*

$$h^2 \cdot [d_y f \| g]_{\rm ew} = -h^2 \cdot \langle f \| D_y g \rangle \,. \tag{3.20}$$

Proposition 3.2.2. (discrete Green's first identity:) *Let* ϕ, $\psi \in m \times n$ *be periodic grid functions. Then*

$$\begin{aligned} h^2 \, [D_x\phi \| D_x\psi]_{\rm ew} \;\; &+ \;\; h^2 \, [D_y\phi \| D_y\psi]_{\rm ns} \\ &= \;\; -h^2 \, (\phi \| \Delta_h \psi) \,. \end{aligned} \tag{3.21}$$

Proposition 3.2.3. (discrete Green's second identity:) *Let* ϕ, $\psi \in \mathcal{C}_{m\times n}$ *be periodic grid functions. Then*

$$h^2 \, (\phi \| \Delta_h \psi) = h^2 \, (\Delta_h \phi \| \psi) \,. \tag{3.22}$$

Now consider the space

$$H := \{ \phi \in \mathcal{C}_{m\times n} | \, (\phi \| \mathbf{1}) = 0 \} \,, \tag{3.23}$$

and equip this space with the bilinear form

$$(\phi_1 \| \phi_2)_H := [D_x\psi_1 \| D_x\psi_2]_{\rm ew} + [D_y\psi_1 \| D_y\psi_2]_{\rm ns} \,, \tag{3.24}$$

for any ϕ_1, $\phi_2 \in H$, where $\psi_i \in \mathcal{C}_{m\times n}$ is the unique solution to

$$\mathcal{L}(\psi_i) = -\Delta_h \psi_i = \phi_i, \quad \psi_i \text{ periodic}, \quad (\psi_i \| \mathbf{1}) = 0. \tag{3.25}$$

The proof of the following can be found in [38].

Proposition 3.2.4. *$(\phi_1\|\phi_2)_H$ is an inner product on the space H. Moreover,*

$$(\phi_1\|\phi_2)_H = \left(\phi_1\middle\|\mathcal{L}^{-1}(\phi_2)\right) = \left(\mathcal{L}^{-1}(\phi_1)\middle\|\phi_2\right). \tag{3.26}$$

Thus

$$\|\phi\|_H := \sqrt{h^2\ (\phi\|\phi)_H} \tag{3.27}$$

defines a norm on H.

3.3 Discrete Periodic Convolution Operator

Here we define a discrete periodic convolution operator on discrete two-dimensional space. Suppose $\phi \in \mathcal{C}_{m\times n}$ is periodic and $\varphi \in \mathcal{V}_{m\times n}$ is periodic. Then the discrete convolution operator $[\varphi \star \phi] : \mathcal{V}_{m\times n} \times \mathcal{C}_{m\times n} \to \mathcal{C}_{m\times n}$ is defined component-wise as

$$[\varphi \star \phi]_{i,j} = h^2 \sum_{k=1}^{m}\sum_{l=1}^{n} \varphi_{k+\frac{1}{2},l+\frac{1}{2}}\phi_{i-k,j-l}\ . \tag{3.28}$$

Notice very carefully that order is important in the definition of the discrete convolution $[\cdot \star \cdot]$

Lemma 3.3.1. *If $\phi,\psi \in \mathcal{C}_{m\times n}$ are periodic, $\varphi \in \mathcal{V}_{m\times n}$ is even and periodic, then*

$$(\phi\|[\varphi\star\psi]) = (\psi\|[\varphi\star\phi])\ . \tag{3.29}$$

Proof. By definition

$$(\phi\|[\varphi\star\psi]) = h^2 \sum_{i=1}^{m}\sum_{j=1}^{n}\phi_{i,j}\sum_{k=1}^{m}\sum_{l=1}^{n}\varphi_{i-k+\frac{1}{2},j-l+\frac{1}{2}}\psi_{k,l}\ . \tag{3.30}$$

Since φ is an even function, for any i,j,k,l

$$\begin{aligned}\varphi_{i-k+\frac{1}{2},j-l+\frac{1}{2}} &= \varphi\left((i-k)\cdot h,(j-l)\cdot h\right)\\ &= \varphi\left((k-i)\cdot h,(l-j)\cdot h\right)\\ &= \varphi_{k-i+\frac{1}{2},l-j+\frac{1}{2}}\ . \end{aligned} \tag{3.31}$$

Thus

$$\begin{aligned}\sum_{i=1}^{m}\sum_{j=1}^{n}\phi_{i,j}\sum_{k=1}^{m}\sum_{l=1}^{n}\varphi_{i-k+\frac{1}{2},j-l+\frac{1}{2}}\psi_{k,l} &= \sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{m}\sum_{l=1}^{n}\phi_{i,j}\varphi_{k-i+\frac{1}{2},l-j+\frac{1}{2}}\psi_{k,l}\\ &= \sum_{k=1}^{m}\sum_{l=1}^{n}\psi_{k,l}\sum_{i=1}^{m}\sum_{j=1}^{n}\varphi_{k-i+\frac{1}{2},l-j+\frac{1}{2}}\phi_{i,j}\ .\end{aligned}$$

By definition,

$$h^2\sum_{k=1}^{m}\sum_{l=1}^{n}\psi_{k,l}\sum_{i=1}^{m}\sum_{j=1}^{n}\varphi_{k-i+\frac{1}{2},l-j+\frac{1}{2}}\phi_{i,j} = (\psi\|[\varphi\star\phi])\ . \tag{3.32}$$

□

Lemma 3.3.2. *If $\phi,\psi\in\mathcal{C}_{m\times n}$ are periodic, $\varphi\in\mathcal{V}_{m\times n}$ is even, positive and periodic, then, for any $\alpha>0$,*

$$|\,(\phi\|[\varphi\star\psi])\,| \le \frac{\alpha}{2}\,[\varphi\star 1]\ (\phi\|\phi) + \frac{1}{2\alpha}\,[\varphi\star 1]\ (\psi\|\psi)\ . \tag{3.33}$$

Proof. By definition,

$$
\begin{aligned}
|\left(\phi\|[\varphi\star\psi]\right)| \leq & h^2 \sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{m}\sum_{l=1}^{n} \varphi_{k+\frac{1}{2},l+\frac{1}{2}} |\phi_{i-k,j-l}\psi_{i,j}| \\
\leq & h^2 \sum_{i=1}^{m}\sum_{j=1}^{n}\sum_{k=1}^{m}\sum_{l=1}^{n} \varphi_{k+\frac{1}{2},l+\frac{1}{2}} \frac{1}{2}\left(\phi_{i-k,j-l}^2 + \psi_{i,j}^2\right) \\
\leq & \frac{\alpha}{2}\left(1\middle\|\left[\varphi\star\phi^2\right]\right) + \frac{1}{2\alpha}\left[\varphi\star 1\right]\left(\psi\|\psi\right) \\
= & \frac{\alpha}{2}\left(\phi^2\middle\|\left[\varphi\star 1\right]\right) + \frac{1}{2\alpha}\left[\varphi\star 1\right]\left(\psi\|\psi\right) \\
= & \frac{\alpha}{2}\left[\varphi\star 1\right]\left(\phi\|\phi\right) + \frac{1}{2\alpha}\left[\varphi\star 1\right]\left(\psi\|\psi\right) \ .
\end{aligned}
$$

□

We remark that these definitions and formulas have straightforward extensions to three dimensions.

3.4 Discrete Identities and Inequalities

In this section we present the two-dimensional version of the identities we proved in Sec. 2.4.

Proposition 3.4.1. *If $\phi, \psi \in \mathcal{C}_{m\times n}$ are periodic, then*

$$
-2h^2\left(\phi\|\Delta_h\psi\right) \leq \|\nabla_h\phi\|_2^2 + \|\nabla_h\psi\|_2^2 \ . \tag{3.34}
$$

Proof. Using summation-by-parts

$$
-2h^2\left(\phi\|\Delta_h\psi\right) = 2h^2\left[D_x\phi\|D_x\psi\right]_{\mathrm{ew}} + 2h^2\left[D_y\phi\|D_y\psi\right]_{\mathrm{ns}} \ . \tag{3.35}
$$

By Young inequality

$$
2h^2\left[D_x\phi\|D_x\psi\right]_{\mathrm{ew}} \leq h^2\left[(D_x\phi)^2\middle\|1\right]_{\mathrm{ew}} + h^2\left[1\middle\|(D_x\psi)^2\right]_{\mathrm{ew}} \ . \tag{3.36}
$$

Similarly

$$2h^2 \left[D_y\phi \| D_y\psi\right]_{\text{ns}} \le h^2 \left[(D_y\phi)^2 \middle\| 1\right]_{\text{ns}} + h^2 \left[1 \middle\| (D_y\psi)^2\right]_{\text{ns}} \ . \tag{3.37}$$

The result follows automatically. □

Lemma 3.4.1. *If $\phi, \psi \in \mathcal{C}_{m\times n}$ are periodic, $(\phi - \psi \| 1) = 0$ and $\|\phi\|_4 < C_1, \|\psi\|_4 < C_2$, and $\|\phi\|_\infty < C_3, \|\nabla_h \phi\|_\infty < C_4$, where C_1, C_2, C_3, C_4 are positive constants independent of h, then there exists a positive constant M_2 which is independent of h, such that*

$$2h^2 \left(\phi^3 - \psi^3 \middle\| \Delta_h (\phi - \psi)\right) \le M_2 \left\|\nabla_h (\phi - \psi)\right\|_2^2 \ . \tag{3.38}$$

Proof. Using summation-by-parts,

$$\begin{aligned} 2h^2 \left(\phi^3 - \psi^3 \middle\| \Delta_h (\phi - \psi)\right) =& - 2h^2 \left[D_x\left(\phi^3 - \psi^3\right) \middle\| D_x (\phi - \psi)\right]_{\text{ew}} \\ & - 2h^2 \left[D_y\left(\phi^3 - \psi^3\right) \middle\| D_y (\phi - \psi)\right]_{\text{ns}} \ . \end{aligned} \tag{3.39}$$

Denote

$$\mathbb{A}_x\phi_{i+\frac{1}{2},j} = \frac{1}{2}\left(\phi_{i+1,j}\right)^2 + \frac{1}{2}\left(\phi_{i,j}\right)^2 + \frac{1}{2}\left(\phi_{i+1,j} + \phi_{i,j}\right)^2 \ , \tag{3.40}$$

and

$$\mathbb{A}_y\phi_{i,j+\frac{1}{2}} = \frac{1}{2}\left(\Phi_{i,j+1}\right)^2 + \frac{1}{2}\left(\Phi_{i,j}\right)^2 + \frac{1}{2}\left(\Phi_{i,j+1} + \Phi_{i,j}\right)^2 \ . \tag{3.41}$$

By definition

$$\begin{aligned} D_x\phi^3_{i+\frac{1}{2},j} =& \frac{1}{h}\left(\phi^3_{i+1,j} - \phi^3_{i,j}\right) = \left[\phi^2_{i+1,j} + \phi^2_{i,j} + \phi_{i+1,j}\phi_{i,j}\right] D_x\phi_{i+\frac{1}{2},j} \\ =& \mathbb{A}_x\phi_{i+\frac{1}{2},j} D_x\phi_{i+\frac{1}{2},j} \ , \\ D_x\psi^3_{i+\frac{1}{2},j} =& \frac{1}{h}\left(\psi^3_{i+1,j} - \psi^3_{i,j}\right) = \left[\psi^2_{i+1,j} + \psi^2_{i,j} + \psi_{i+1,j}\psi_{i,j}\right] D_x\psi_{i+\frac{1}{2},j} \\ =& \mathbb{A}_x\psi_{i+\frac{1}{2},j} D_x\psi_{i+\frac{1}{2},j} \ . \end{aligned} \tag{3.42}$$

Thus

$$- \left[D_x\left(\phi^3 - \psi^3\right) \middle\| D_x (\phi - \psi)\right]_{\text{ew}} = - \left[\mathbb{A}_x\phi D_x\phi - \mathbb{A}_x\psi D_x\psi \| D_x (\phi - \psi)\right]_{\text{ew}} \ . \tag{3.43}$$

By adding and subtracting $\mathbb{A}_x\psi D_x\phi$, we have

$$
\begin{aligned}
-2h^2 \left[D_x\left(\phi^3-\psi^3\right)\middle\| D_x(\phi-\psi)\right]_{\mathrm{ew}} =& -2h^2\left[\mathbb{A}_x\phi D_x\phi-\mathbb{A}_x\psi D_x\phi \| D_x(\phi-\psi)\right]_{\mathrm{ew}} \\
& -2h^2\left[\mathbb{A}_x\psi D_x\phi-\mathbb{A}_x\psi D_x\psi \| D_x(\phi-\psi)\right]_{\mathrm{ew}} .
\end{aligned} \tag{3.44}
$$

Noticing that

$$
\left[\mathbb{A}_x\psi D_x\phi-\mathbb{A}_x\psi D_x\psi \| D_x(\phi-\psi)\right]_{\mathrm{ew}} = \left[\mathbb{A}_x\psi\middle\|\left(D_x(\phi-\psi)\right)^2\right]_{\mathrm{ew}} . \tag{3.45}
$$

This together with $\mathbb{A}_x\psi \geq 0$ yields

$$
\begin{aligned}
-2h^2 \left[D_x\left(\phi^3-\psi^3\right)\middle\| D_x(\phi-\psi)\right]_{\mathrm{ew}} \leq& -2h^2\left[\left(\mathbb{A}_x\phi-\mathbb{A}_x\psi\right) D_x\phi \| D_x(\phi-\psi)\right]_{\mathrm{ew}} \\
\leq& 2h^2\left|\left[\left(\mathbb{A}_x\phi-\mathbb{A}_x\psi\right) D_x\phi \| D_x(\phi-\psi)\right]_{\mathrm{ew}}\right| \\
\leq& 2h^2\left[\left(\left|\mathbb{A}_x\phi-\mathbb{A}_x\psi\right|\right)\left(\left|D_x\phi\right|\right) \| \left(\left|D_x(\phi-\psi)\right|\right)\right]_{\mathrm{ew}} .
\end{aligned} \tag{3.46}
$$

Since $\|\phi\|_\infty < C_3$, $\|\nabla_h\phi\|_\infty < C_4$,

$$
-2h^2 \left[D_x\left(\phi^3-\psi^3\right)\middle\| D_x(\phi-\psi)\right]_{\mathrm{ew}} \leq 2h^2 C_4\left[\left(\left|\mathbb{A}_x\phi-\mathbb{A}_x\psi\right|\right) \| \left(\left|D_x(\phi-\psi)\right|\right)\right]_{\mathrm{ew}} . \tag{3.47}
$$

By Hölder inequality, we obtain

$$
\begin{aligned}
& 2h^2\left[\left(\left|\mathbb{A}_x\phi-\mathbb{A}_x\psi\right|\right) \| \left(\left|D_x(\phi-\psi)\right|\right)\right]_{\mathrm{ew}} \\
\leq& 2h^2\left[\left(\mathbb{A}_x\phi-\mathbb{A}_x\psi\right)^2\middle\| 1\right]_{\mathrm{ew}}^{\frac{1}{2}}\left[1\middle\|\left(D_x(\phi-\psi)\right)^2\right]_{\mathrm{ew}}^{\frac{1}{2}} .
\end{aligned} \tag{3.48}
$$

Also noticing that

$$
\begin{aligned}
&(\mathbb{A}_x\phi - \mathbb{A}_x\psi)_{i+\frac{1}{2},j} \\
=&\frac{1}{2}\phi_{i+1,j}^2 + \frac{1}{2}\phi_{i,j}^2 + \frac{1}{2}\left(\phi_{i+1,j} + \phi_{i,j}\right)^2 \\
&- \frac{1}{2}\psi_{i+1,j}^2 - \frac{1}{2}\psi_{i,j}^2 - \frac{1}{2}\left(\phi_{i+1,j} + \phi_{i,j}\right)^2 \\
=&\frac{1}{2}\left(\phi_{i+1,j} + \psi_{i+1,j}\right)\left(\phi_{i+1,j} - \psi_{i+1,j}\right) + \frac{1}{2}\left(\phi_{i,j} + \psi_{i,j}\right)\left(\phi_{i,j} - \psi_{i,j}\right) \\
&+ \frac{1}{2}\left(\phi_{i+1,j} + \psi_{i+1,j} + \phi_{i,j} + \psi_{i,j}\right)\left(\phi_{i+1,j} - \psi_{i+1,j} + \phi_{i,j} - \psi_{i,j}\right) \ . \qquad (3.49)
\end{aligned}
$$

Thus

$$
\begin{aligned}
&(\mathbb{A}_x\phi - \mathbb{A}_x\psi)_{i+\frac{1}{2},j}^2 \\
\leq&\frac{3}{4}\left(\phi_{i+1,j} + \psi_{i+1,j}\right)^2\left(\phi_{i+1,j} - \psi_{i+1,j}\right)^2 + \frac{3}{4}\left(\phi_{i,j} + \psi_{i,j}\right)^2\left(\phi_{i,j} - \psi_{i,j}\right)^2 \\
&+ \frac{3}{4}\left(\phi_{i+1,j} + \psi_{i+1,j} + \phi_{i,j} + \psi_{i,j}\right)^2\left(\phi_{i+1,j} - \psi_{i+1,j} + \phi_{i,j} - \psi_{i,j}\right)^2 \\
\leq&\frac{3}{4}\left(\phi_{i+1,j} + \psi_{i+1,j}\right)^2\left(\phi_{i+1,j} - \psi_{i+1,j}\right)^2 + \frac{3}{4}\left(\phi_{i,j} + \psi_{i,j}\right)^2\left(\phi_{i,j} - \psi_{i,j}\right)^2 \\
&+ 3\left(\left(\phi_{i+1,j} + \psi_{i+1,j}\right)^2 + \left(\phi_{i,j} + \psi_{i,j}\right)^2\right)\left(\left(\phi_{i+1,j} - \psi_{i+1,j}\right)^2 + \left(\phi_{i,j} - \psi_{i,j}\right)^2\right) \\
\leq&\frac{15}{4}\left(\left(\phi_{i+1,j} + \psi_{i+1,j}\right)^2 + \left(\phi_{i,j} + \psi_{i,j}\right)^2\right)\left(\left(\phi_{i+1,j} - \psi_{i+1,j}\right)^2 + \left(\phi_{i,j} - \psi_{i,j}\right)^2\right) \ . \qquad (3.50)
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
&(\mathbb{A}_x\phi - \mathbb{A}_x\psi)_{i-\frac{1}{2},j}^2 \\
\leq&\frac{15}{4}\left(\left(\phi_{i-1,j} + \psi_{i-1,j}\right)^2 + \left(\phi_{i,j} + \psi_{i,j}\right)^2\right)\left(\left(\phi_{i-1,j} - \psi_{i-1,j}\right)^2 + \left(\phi_{i,j} - \psi_{i,j}\right)^2\right) \ . \qquad (3.51)
\end{aligned}
$$

Denote

$$
\mathbb{H}_{i+\frac{1}{2},j} = \frac{1}{2}\left(\left(\phi_{i+1,j} + \psi_{i+1,j}\right)^2 + \left(\phi_{i,j} + \psi_{i,j}\right)^2\right) \ , \qquad (3.52)
$$

$$
\mathbb{G}_{i+\frac{1}{2},j} = \frac{1}{2}\left(\left(\phi_{i+1,j} - \psi_{i+1,j}\right)^2 + \left(\phi_{i,j} - \psi_{i,j}\right)^2\right) . \qquad (3.53)
$$

By the definition of $[\cdot\|\cdot]_{\mathrm{ew}}$ and Hölder inequality, we see that

$$\begin{aligned}\left[(\mathbb{A}_x\phi - \mathbb{A}_x\psi)^2\middle\|1\right]_{\mathrm{ew}} \leq & 15\,[\mathbb{H}\|\mathbb{G}]_{\mathrm{ew}} \\ \leq & 15\left[\mathbb{H}^2\middle\|1\right]_{\mathrm{ew}}^{\frac{1}{2}}\left[1\middle\|\mathbb{G}^2\right]_{\mathrm{ew}}^{\frac{1}{2}} \ .\end{aligned} \tag{3.54}$$

The definition of $\mathbb{H}_{i+\frac{1}{2},j}$ shows that

$$\begin{aligned}\mathbb{H}^2_{i+\frac{1}{2},j} = & \frac{1}{4}\left((\phi_{i+1,j}+\psi_{i+1,j})^2 + (\phi_{i,j}+\psi_{i,j})^2\right)^2 \\ \leq & 4\left((\phi_{i+1,j})^4 + (\psi_{i+1,j})^4 + (\phi_{i,j})^4 + (\psi_{i,j})^4\right) \ .\end{aligned} \tag{3.55}$$

By the definition of $[\cdot\|\cdot]_{\mathrm{ew}}$ and the periodic boundary condition, we get

$$\left[\mathbb{H}^2\middle\|1\right]_{\mathrm{ew}} \leq \frac{1}{2h^2}\|\phi\|_4^4 + \frac{1}{2h^2}\|\psi\|_4^4 \ . \tag{3.56}$$

Similarly

$$\left[1\middle\|\mathbb{G}^2\right]_{\mathrm{ew}} \leq \frac{1}{h^2}\|\phi-\psi\|_4^4 \ . \tag{3.57}$$

Thus

$$\left[(\mathbb{A}_x\phi - \mathbb{A}_x\psi)^2\middle\|1\right]_{\mathrm{ew}} \leq \frac{1}{h}\left[1800\left(\|\phi\|_4^4 + \|\psi\|_4^4\right)\right]^{\frac{1}{2}}\|\phi-\psi\|_4^2 \ . \tag{3.58}$$

Also

$$\left[(D_x(\phi-\psi))^2\middle\|1\right]_{\mathrm{ew}}^{\frac{1}{2}} = \frac{1}{h}\|D_x(\phi-\psi)\|_2 \ . \tag{3.59}$$

Combining the above results,

$$\begin{aligned} & -2h^2\left[D_x\left(\phi^3-\psi^3\right)\middle\|D_x(\phi-\psi)\right]_{\mathrm{ew}} \\ \leq & 2C_4\left[1800\left(\|\phi\|_4^4+\|\psi\|_4^4\right)\right]^{\frac{1}{4}}\|\phi-\psi\|_4\|D(\phi-\psi)\|_2 \ .\end{aligned} \tag{3.60}$$

With the same method we can also prove that

$$\begin{aligned}
&-2h^2\left[D_y\left(\phi^3-\psi^3\right)\middle\| D_y\left(\phi-\psi\right)\right]_{\text{ns}}\\
&\leq 2C_4\left[1800\left(\|\phi\|_4^4+\|\psi\|_4^4\right)\right]^{\frac{1}{4}}\|\phi-\psi\|_4\left\|D\left(\phi-\psi\right)\right\|_2\ . \qquad (3.61)
\end{aligned}$$

We borrowed a lemma proved from [38] which yields that under the condition $(\phi-\psi|1)=0$,

$$\|\phi-\psi\|_4\leq C_5\left\|D\left(\phi-\psi\right)\right\|_2\ , \qquad (3.62)$$

where C_5 is a constant independent of h. Therefore

$$2h\left(\phi^3-\psi^3\middle|\Delta_h\left(\phi-\psi\right)\right)\leq 4\left[1800\left(\|\phi\|_4^4+\|\psi\|_4^4\right)\right]^{\frac{1}{4}}C_4C_5\left\|D\left(\phi-\psi\right)\right\|_2^2\ . \qquad (3.63)$$

By the assumption of $\|\phi\|_4$ and $\|\psi\|_4$, the result follows. □

Lemma 3.4.2. *If $\phi\in\mathcal{C}_{m\times n}$ is periodic, J is defined as (J1 - J3) and $J_{i+\frac{1}{2},j+\frac{1}{2}}:=J(x_{i+\frac{1}{2}},y_{j+\frac{1}{2}})$. Then for any $\alpha_2>0$*

$$-2h^2\left(\left[J\star\phi\right]\|\Delta_h\phi\right)\leq M_{11}\frac{1}{\alpha_2}\|\phi\|_2^2+\alpha_2\left\|\nabla_h\phi\right\|_2^2\ , \qquad (3.64)$$

where M_{11} is a positive constant independent of h.

Proof. Using summation-by-parts and Young inequality

$$\begin{aligned}
-2h^2\left(\left[J\star\phi\right]\|\Delta_h\phi\right)=&2h^2\left[D_x\left[J\star\phi\right]\|D_x\phi\right]_{\text{ew}}+2h^2\left[D_y\left[J\star\phi\right]\|D_y\phi\right]_{\text{ns}}\\
\leq&\frac{h^2}{\alpha_2}\left[\left(D_x\left[J\star\phi\right]\right)^2\middle\|1\right]_{\text{ew}}+\alpha_2h^2\left[1\middle\|\left(D_x\phi\right)^2\right]_{\text{ew}}\\
&+\frac{h^2}{\alpha_2}\left[\left(D_y\left[J\star\phi\right]\right)^2\middle\|1\right]_{\text{ns}}+\alpha_2h^2\left[1\middle\|\left(D_y\phi\right)^2\right]_{\text{ns}}\ . \qquad (3.65)
\end{aligned}$$

By the definition of discrete operator, we have

$$\begin{aligned} D_x \left[J \star \phi\right]_{i+\frac{1}{2},j} =& \frac{1}{h}\left(h^2 \sum_{k=1}^{m}\sum_{l=1}^{n} J_{(i+1)-k+\frac{1}{2},j-l+\frac{1}{2}}\phi_{k,l} - h^2 \sum_{k=1}^{m}\sum_{l=1}^{n} J_{i-k+\frac{1}{2},j-l+\frac{1}{2}}\phi_{k,l}\right) \\ =& h^2 \sum_{k=1}^{m}\sum_{l=1}^{n} \frac{1}{h}\left(J_{(i+1)-k+\frac{1}{2},j-l+\frac{1}{2}} - J_{i-k+\frac{1}{2},j-l+\frac{1}{2}}\right)\phi_{k,l} \\ =& h^2 \sum_{k=1}^{m}\sum_{l=1}^{n} \left(d_x J_{i-k+\frac{1}{2},j-l+\frac{1}{2}}\right)\phi_{k,l} \ . \end{aligned} \tag{3.66}$$

By the definition of J there exists a constant C independent of h, such that $\|\nabla_h J\|_\infty < C$. Therefore

$$D_x \left[J \star \phi\right]_{i+\frac{1}{2},j} \leq C h^2 \sum_{k=1}^{m}\sum_{l=1}^{n} \phi_{k,l} \ . \tag{3.67}$$

Thus by discrete Hölder inequality

$$\begin{aligned} \left(D_x \left[J \star \phi\right]_{i+\frac{1}{2},j}\right)^2 \leq& C^2 h^4 \left(\sum_{k=1}^{m}\sum_{l=1}^{n} \phi_{k,l}\right)^2 \leq C^2 h^4 mn \sum_{k=1}^{m}\sum_{l=1}^{n} \left(\phi_{k,l}\right)^2 \\ =& C^2 h^2 |\Omega| \, \|\phi\|_2^2 \ . \end{aligned} \tag{3.68}$$

Therefore

$$\frac{h^2}{\alpha_2}\left[(D_x \left[J \star \phi\right])^2 \middle\| 1\right]_{\text{ew}} \leq \frac{C^2 |\Omega|^2}{\alpha_2} \|\phi\|_2^2 \ . \tag{3.69}$$

Similarly

$$\frac{h^2}{\alpha_2}\left[(D_y \left[J \star \phi\right])^2 \middle\| 1\right]_{\text{ns}} \leq \frac{C^2 |\Omega|^2}{\alpha_2} \|\phi\|_2^2 \ . \tag{3.70}$$

The result follows immediately. □

3.5 Cut-off Functions and Their Properties

In this section we are going to discuss the two-dimensional estimates of cut-off function in Sec. 2.5. Since the cut-off function proposed in that section can works for two-dimensional as well, we will just use the result of Prop. 2.5.1 directly.

Lemma 3.5.1. *If $\phi, \psi \in \mathcal{C}_{m\times n}$ are periodic, and $\|\phi\|_\infty < C_3$, $\|\nabla_h \phi\|_\infty < C_4$, where C_3, C_4 are positive constants independent of h. Let $M_3 > 0$ be given and F_{M_3} is as defined in Eq. (2.41), then for any $\alpha_1 > 0$*

$$2h^2 \left(F_{M_3}(\phi) - F_{M_3}(\psi) \| \Delta_h (\phi - \psi)\right) \leq \frac{M_7}{\alpha_1} \|\phi - \psi\|_2^2 + \alpha_1 M_8 \|\nabla_h (\phi - \psi)\|_2^2 + \frac{M_9}{\alpha_1} h^4, \tag{3.71}$$

where M_7, M_8 and M_9 are positive constants independent of h, but depend on M_3.

Proof. Using summation-by-parts, we have

$$\begin{aligned} 2h^2 \left(F_{M_3}(\phi) - F_{M_3}(\psi) \| \Delta_h (\phi - \psi)\right) = &- 2h^2 \left[D_x \left(F_{M_3}(\phi) - F_{M_3}(\phi)\right) \| D_x (\phi - \psi)\right]_{\mathrm{ew}} \\ &- 2h^2 \left[D_y \left(F_{M_3}(\phi) - F_{M_3}(\phi)\right) \| D_y (\phi - \psi)\right]_{\mathrm{ns}} . \end{aligned} \tag{3.72}$$

Denote

$$\begin{aligned} \delta_h F_{M_3}(\phi)_{i+\frac{1}{2},j} &= \frac{\left[F_{M_3}(\phi_{i+1,j}) - F_{M_3}(\phi_{i,j})\right]}{\left[\phi_{i+1,j} - \phi_{i,j}\right]}, \\ \delta_h F_{M_3}(\psi)_{i+\frac{1}{2},j} &= \frac{\left[F_{M_3}(\psi_{i+1,j}) - F_{M_3}(\psi_{i,j})\right]}{\left[\psi_{i+1,j} - \psi_{i,j}\right]}. \end{aligned} \tag{3.73}$$

Since F_{M_3} is increasing, $\delta_h F_{M_3}(\phi) \geq 0$, $\delta_h F_{M_3}(\psi) \geq 0$. An application of Taylor expansion shows that

$$\begin{aligned} F_{M_3}(\phi_{i+1,j}) - F_{M_3}(\phi_{i,j}) =& F'_{M_3}(\phi_{i,j})(\phi_{i+1,j} - \phi_{i,j}) \\ &+ \frac{1}{2} F''_{M_3}(\xi_{i,j})(\phi_{i+1,j} - \phi_{i,j})^2, \quad \xi_{i,j} \in [\phi_{i,j}, \phi_{i+1,j}] \ . \end{aligned} \tag{3.74}$$

By definition,

$$\begin{aligned} D_x F_{M_3}(\phi)_{i+\frac{1}{2},j} =& \frac{1}{h}\left[F_{M_3}(\phi_{i+1,j}) - F_{M_3}(\phi_{i,j})\right] \\ =& \frac{\left[F_{M_3}(\phi_{i+1,j}) - F_{M_3}(\phi_{i,j})\right]}{\left[\phi_{i+1,j} - \phi_{i,j}\right]} \frac{\left[\phi_{i+1,j} - \phi_{i,j}\right]}{h} \\ =& \delta_h F_{M_3}(\phi)_{i+\frac{1}{2},j} D_x \phi_{i+\frac{1}{2},j} \ . \end{aligned} \tag{3.75}$$

Similarly,

$$D_x F_{M_3}(\psi)_{i+\frac{1}{2},j} = \delta_h F_{M_3}(\psi)_{i+\frac{1}{2},j} D\psi_{i+\frac{1}{2},j} \ . \tag{3.76}$$

Thus

$$\begin{aligned} & -2h^2 \left[D_x \left(F_{M_3}(\phi) - F_{M_3}(\psi)\right) \| D_x(\phi - \psi)\right]_{\text{ew}} \\ =& -2h^2 \left[\delta_h F_{M_3}(\phi) D_x \phi - \delta_h F_{M_3}(\psi) D_x \psi \| D_x(\phi - \psi)\right]_{\text{ew}} \ . \end{aligned} \tag{3.77}$$

By adding and subtracting $\delta_h F_{M_3}(\psi) D\phi$,

$$\begin{aligned} & -2h^2 \left[D_x \left(F_{M_3}(\phi) - F_{M_3}(\psi)\right) \| D_x(\phi - \psi)\right]_{\text{ew}} \\ =& -2h^2 \left[\delta_h F_{M_3}(\phi) D_x \phi - \delta_h F_{M_3}(\psi) D_x \phi \| D_x(\phi - \psi)\right]_{\text{ew}} \\ & -2h^2 \left[\delta_h F_{M_3}(\psi) D_x \phi - \delta_h F_{M_3}(\psi) D_x \psi \| D_x(\phi - \psi)\right]_{\text{ew}} \ . \end{aligned}$$

Notice that

$$
\begin{aligned}
&-2h^2\left[\delta_h F_{M_3}(\psi)\, D_x\phi - \delta_h F_{M_3}(\psi)\, D_x\psi \| D_x(\phi-\psi)\right]_{\mathrm{ew}} \\
=&-2h^2\left[\delta_h F_{M_3}(\psi) \| \left(D_x(\phi-\psi)\right)^2\right]_{\mathrm{ew}} \ .
\end{aligned} \tag{3.78}
$$

This together with $\delta_h F_{M_3}(\psi) \geq 0$ yields

$$
\begin{aligned}
&-2h^2\left[D_x\left(F_{M_3}(\phi) - F_{M_3}(\psi)\right) \| D_x(\phi-\psi)\right]_{\mathrm{ew}} \\
\leq&-2h^2\left[\left(\delta_h F_{M_3}(\phi) - \delta_h F_{M_3}(\psi)\right) D_x\phi \| D_x(\phi-\psi)\right]_{\mathrm{ew}} \\
\leq&2h^2\left|\left[\left(\delta_h F_{M_3}(\phi) - \delta_h F_{M_3}(\psi)\right) D_x\phi \| D_x(\phi-\psi)\right]_{\mathrm{ew}}\right| \\
\leq&2h^2\left[\left(\left|\delta_h F_{M_3}(\phi) - \delta_h F_{M_3}(\psi)\right|\right)\left(\left|D_x\phi\right|\right) \| \left(\left|D_x(\phi-\psi)\right|\right)\right]_{\mathrm{ew}} \ .
\end{aligned} \tag{3.79}
$$

By the fact that $\|\phi\|_\infty < C_3$, $\|D\phi\|_\infty < C_4$, we get

$$
\begin{aligned}
&-2h^2\left[D_x\left(F_{M_3}(\phi) - F_{M_3}(\psi)\right) \| D_x(\phi-\psi)\right]_{\mathrm{ew}} \\
\leq&2h^2 C_4\left[\left(\left|\delta_h F_{M_3}(\phi) - \delta_h F_{M_3}(\psi)\right|\right) \| \left(\left|D_x(\phi-\psi)\right|\right)\right]_{\mathrm{ew}} \ .
\end{aligned} \tag{3.80}
$$

By the Taylor expansion,

$$
\begin{aligned}
&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2},j} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2},j}\right| \\
=&\left|\frac{F'_{M_3}(\phi_{i,j})\left(\phi_{i+1,j}-\phi_{i,j}\right) + \frac{1}{2}F''_{M_3}(\xi_{i,j})\left(\phi_{i+1,j}-\phi_{i,j}\right)^2}{\phi_{i+1,j}-\phi_{i,j}}\right. \\
&\left.-\frac{F'_{M_3}(\psi_{i,j})\left(\psi_{i+1,j}-\psi_{i,j}\right) + \frac{1}{2}F''_{M_3}(\eta_{i,j})\left(\psi_{i+1,j}-\psi_{i,j}\right)^2}{\psi_{i+1,j}-\psi_{i,j}}\right| \\
\leq&\left|F'_{M_3}(\phi_{i,j}) - F'_{M_3}(\psi_{i,j})\right| + \frac{1}{2}\left|F''_{M_3}(\xi_{i,j})\left(\phi_{i+1,j}-\phi_{i,j}\right) - F''_{M_3}(\eta_{i,j})\left(\psi_{i+1,j}-\psi_{i,j}\right)\right| \ .
\end{aligned} \tag{3.81}
$$

By Prop. 2.5.1, it is easy to prove F'_{M_3} is Lipschitz continuous. Thus

$$\begin{aligned}&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2},j} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2},j}\right| \\ \leq & 6M_3\left|\phi_{i,j} - \psi_{i,j}\right| + \frac{1}{2}\left|F''_{M_3}(\xi_{i,j})(\phi_{i+1,j} - \phi_{i,j}) - F''_{M_3}(\eta_{i,j})(\psi_{i+1,j} - \psi_{i,j})\right|. \end{aligned} \tag{3.82}$$

Notice that

$$\begin{aligned}&\left|F''_{M_3}(\xi_{i,j})(\phi_{i+1,j} - \phi_{i,j}) - F''_{M_3}(\eta_{i,j})(\psi_{i+1,j} - \psi_{i,j})\right| \\ = & \left|F''_{M_3}(\xi_{i,j})\phi_{i+1,j} - F''_{M_3}(\xi_{i,j})\phi_{i,j} - F''_{M_3}(\eta_{i,j})\psi_{i+1,j} + F''_{M_3}(\eta_{i,j})\psi_{i,j}\right|. \end{aligned} \tag{3.83}$$

Adding and subtracting $F''_{M_3}(\eta_{i,j})\phi_{i+1,j}$ and $F''_{M_3}(\xi_{i,j})\psi_{i,j}$ gives

$$\begin{aligned}&\left|F''_{M_3}(\xi_{i,j})(\phi_{i+1,j} - \phi_{i,j}) - F''_{M_3}(\eta_{i,j})(\psi_{i+1,j} - \psi_{i,j})\right| \\ = & \left| \left[F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right]\phi_{i+1,j} + F''_{M_3}(\eta_{i,j})\left[\phi_{i+1,j} - \psi_{i+1,j}\right] \right. \\ & \left. - \left[F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right]\psi_{i,j} - F''_{M_3}(\xi_{i,j})\left[\phi_{i,j} - \psi_{i,j}\right]\right| \\ \leq & \left|F''_{M_3}(\eta_{i,j})\left[\phi_{i+1,j} - \psi_{i+1,j}\right]\right| + \left|F''_{M_3}(\xi_{i,j})\left[\phi_{i,j} - \psi_{i,j}\right]\right| \\ & + \left| \left[F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right]\right|\left|\phi_{i+1,j} - \psi_{i,j}\right|. \end{aligned} \tag{3.84}$$

By the property of F''_{M_3}, $F''_{M_3} \leq 12M_3$,

$$\begin{aligned}&\left|F''_{M_3}(\xi_{i,j})(\phi_{i+1,j} - \phi_{i,j}) - F''_{M_3}(\eta_{i,j})(\psi_{i+1,j} - \psi_{i,j})\right| \\ \leq & 12M_3\left|\phi_{i+1,j} - \psi_{i+1,j}\right| + 12M_3\left|\phi_{i,j} - \psi_{i,j}\right| + \left| \left[F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right]\right|\left|\phi_{i+1,j} - \psi_{i,j}\right|. \end{aligned} \tag{3.85}$$

Furthermore, adding and subtracting $\phi_{i,j}$ yields

$$\begin{aligned}
&\left| \left[F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right] \right| \left|\phi_{i+1,j} - \psi_{i,j}\right| \\
=&\left| \left[F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right] \right| \left|\phi_{i+1,j} - \phi_{i,j} + \phi_{i,j} - \psi_{i,j}\right| \\
\leq&\left|F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right| \left|\phi_{i+1,j} - \phi_{i,j}\right| + \left|F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right| \left|\phi_{i,j} - \psi_{i,j}\right| \\
\leq&\left|F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right| \left|\phi_{i+1,j} - \phi_{i,j}\right| + 24M_3\left|\phi_{i,j} - \psi_{i,j}\right| \ . \qquad (3.86)
\end{aligned}$$

By multiplying and dividing h, $\phi_{i+1,j} - \phi_{i,j} = hD\phi_{i+\frac{1}{2},j}$, together with the Lipschitz continuity of F''_{M_3}, we have

$$\left|F''_{M_3}(\xi_{i,j}) - F''_{M_3}(\eta_{i,j})\right| \left|\phi_{i+1,j} - \phi_{i,j}\right| \leq 6M_3hC_4\left|\xi_{i,j} - \eta_{i,j}\right| \ . \qquad (3.87)$$

By the definition of $\xi_{i,j}$ and $\eta_{i,j}$,

$$\begin{aligned}
\left|\xi_{i,j} - \eta_{i,j}\right| \leq&\left|\phi_{i+1,j} - \psi_{i+1,j}\right| + \left|\phi_{i,j} - \psi_{i,j}\right| + \left|\phi_{i+1,j} - \psi_{i,j}\right| + \left|\phi_{i,j} - \psi_{i+1,j}\right| \\
\leq&\left|\phi_{i+1,j} - \psi_{i+1,j}\right| + \left|\phi_{i,j} - \psi_{i,j}\right| + \left|\phi_{i+1,j} - \phi_{i,j}\right| \\
&+ \left|\phi_{i,j} - \psi_{i,j}\right| + \left|\phi_{i,j} - \phi_{i+1,j}\right| + \left|\phi_{i+1,j} - \psi_{i+1,j}\right| \\
\leq&2\left|\phi_{i+1,j} - \psi_{i+1,j}\right| + 2\left|\phi_{i,j} - \psi_{i,j}\right| + 2hC_4 \ . \qquad (3.88)
\end{aligned}$$

Combining the above results,

$$\begin{aligned}
&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2},j} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2},j}\right| \\
\leq&6M_3|\phi_{i,j} - \psi_{i,j}| + 6M_3|\phi_{i+1,j} - \psi_{i+1,j}| + 6M_3|\phi_{i,j} - \psi_{i,j}| + 12M_3|\phi_{i,j} - \psi_{i,j}| \\
&+ 6M_3hC_4\left(|\phi_{i+1,j} - \psi_{i+1,j}| + |\phi_{i,j} - \psi_{i,j}| + hC_4\right) \ . \qquad (3.89)
\end{aligned}$$

Without lose of generality, we can assume that h is small. Thus

$$
\begin{aligned}
&\left|\delta_h F_{M_3}(\phi)_{i+\frac{1}{2},j} - \delta_h F_{M_3}(\psi)_{i+\frac{1}{2},j}\right| \\
\leq & 48M_3\left(\frac{1}{2}|\phi_{i+1,j} - \psi_{i+1,j}| + \frac{1}{2}|\phi_{i,j} - \psi_{i,j}|\right) + 6M_3\|D\phi\|_\infty^2 h^2 \\
= & 48M_3\left(A|\phi - \psi|_{i+\frac{1}{2},j}\right) + 6M_3C_4^2h^2 \ . \qquad (3.90)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
& -2h^2\left[D_x\left(F_{M_3}(\phi) - F_{M_3}(\phi)\right)\|D_x(\phi - \psi)\right]_{\mathrm{ew}} \\
\leq & 2h^2C_4\left[48M_3\left(A|\phi - \psi|\right) + 6M_3C_4^2h^2\|(|D_x(\phi - \psi)|)\right]_{\mathrm{ew}} \ . \qquad (3.91)
\end{aligned}
$$

By Cauchy inequality and the definition of $[\cdot\|\cdot]_{\mathrm{ew}}$, we arrive at

$$
\begin{aligned}
& -2h^2\left[D_x\left(F_{M_3}(\phi) - F_{M_3}(\phi)\right)\|D_x(\phi - \psi)\right]_{\mathrm{ew}} \\
\leq & 2h^2C_4\frac{4}{\alpha_1}(48M_3)^2\left[(A|\phi - \psi|)^2\|1\right]_{\mathrm{ew}} + 2h^2C_4\frac{4}{\alpha_1}\left(6M_3C_4^2\right)^2\left[h^4\|1\right]_{\mathrm{ew}} \\
& + 2h^2C_4\frac{\alpha_1}{2}\left[1\|(D_x(\phi - \psi))^2\right]_{\mathrm{ew}} \\
\leq & 2C_4\frac{4}{\alpha_1}(48M_3)^2\|\phi - \psi\|_2^2 + 2C_4\frac{\alpha_1}{2}\|D_x(\phi - \psi)\|_2^2 + 2C_4\frac{4}{\alpha_1}\left(6M_3C_4^2\right)^2|\Omega|h^4. \qquad (3.92)
\end{aligned}
$$

By the same method

$$
\begin{aligned}
& -2h^2\left[D_y\left(F_{M_3}(\phi) - F_{M_3}(\phi)\right)\|D_y(\phi - \psi)\right]_{\mathrm{ns}} \\
\leq & 2C_4\frac{4}{\alpha_1}(48M_3)^2\|\phi - \psi\|_2^2 + 2C_4\frac{\alpha_1}{2}\|D_y(\phi - \psi)\|_2^2 + 2C_4\frac{4}{\alpha_1}\left(6M_3C_4^2\right)^2|\Omega|h^4. \qquad (3.93)
\end{aligned}
$$

Thus the proof follows. □

Chapter 4

First Order (In Time) Schemes and Their Properties

4.1 Overview

Our principal goal in this section is to describe fully discrete, first order in time, second order in space convex splitting schemes for nCH and nAC equations. We will present one part of our main results in this chapter: the unconditional solvability of the scheme, *i.e.* the existence and uniqueness of the solution for the scheme is independent of the time step size s; the unconditional energy stability, *i.e.* the decreasing of the discrete version of energy (1.13) independent of the time step size s and the convergence of the scheme. The main difficulty in this result is that we don't have L^∞ bounds for the numerical solution, therefore in the proof of the convergence of the scheme some unique techniques are applied. Here we are going to only present the convergence proof for scheme of nCH equation. But it need to be noted that the convergence of scheme of nAC equation can be derived easily with the same method.

The chapter will be organized in following way: in Sec. 4.2 we present the first order in time, continuous in space scheme as the motivation, the energy decreasing property will also be discussed; in Sec. 4.3 we define the discrete version of energy 1.13

and discuss its upper bounds, also a discrete pseudo energy is defined for the sake of future second order scheme; in Sec. 4.4 we form the fully discrete first order scheme; in Sec. 4.5 we prove the unconditional unique solvability; in Sec. 4.6 we prove the unconditional energy stability and L^p stability; in Sec. 4.7 the convergence of the scheme for nCH will be discussed.

4.2 The First-Order (In Time) Convex Splitting Scheme

Based on LEM 1.2.2 a first-order (in time) convex splitting scheme for the nCH equation (1.2) can be constructed as follows: given $\phi^k \in C_p^\infty(\Omega)$, find ϕ^{k+1}, $w^{k+1} \in C_p^\infty(\Omega)$ such that

$$\phi^{k+1} - \phi^k = s\Delta w^{k+1}, \tag{4.1}$$

$$\begin{aligned} w^{k+1} &= \left(\phi^{k+1}\right)^3 + \left(2(J_c * 1) + \gamma_c\right)\phi^{k+1} \\ &\quad - \left((J_c * 1) + (J_e * 1) + \gamma_e\right)\phi^k - J * \phi^k \ , \end{aligned} \tag{4.2}$$

where $s > 0$ is the time step size. Similarly, the first-order (in time) convex splitting scheme for the nAC equation (1.3) can be constructed as follows: given $\phi^k \in C_p^\infty(\Omega)$, find ϕ^{k+1}, $w^{k+1} \in C_p^\infty(\Omega)$ such that

$$\phi^{k+1} - \phi^k = -sw^{k+1}, \tag{4.3}$$

$$\begin{aligned} w^{k+1} &= \left(\phi^{k+1}\right)^3 + \left(2(J_c * 1) + \gamma_c\right)\phi^{k+1} \\ &\quad - \left((J_c * 1) + (J_e * 1) + \gamma_e\right)\phi^k - J * \phi^k \ . \end{aligned} \tag{4.4}$$

Notice that this scheme respects the convex splitting of the energy E. The contribution to the chemical potential corresponding to the convex energy E_c is treated implicitly, the part corresponding to the concave part E_e is treated explicitly. We have the following *a priori* energy law for the solutions of the first-order scheme.

Theorem 4.1. *Suppose the energy* $E(\phi)$ *is as defined in Eq. (1.12).* ϕ^{k+1}, $w^{k+1} \in C_p^\infty(\Omega)$ *are pair of solutions to the nCH scheme (4.1) – (4.2). Then for any* $s > 0$,

$$E\left(\phi^{k+1}\right) + s\left\|\nabla w^{k+1}\right\|_{L^2}^2 + R_1^c\left(\phi^k, \phi^{k+1}\right) = E\left(\phi^k\right) \ , \tag{4.5}$$

where

$$\begin{aligned} R_1^c\left(\phi^k, \phi^{k+1}\right) &= \frac{1}{4}\left\|\left(\phi^{k+1}\right)^2 - \left(\phi^k\right)^2\right\|_{L^2}^2 + \frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1} - \phi^k\right)\right\|_{L^2}^2 \\ &+ \frac{\left(3J_c * 1 + J_e * 1 + \gamma_c + \gamma_e\right)}{2}\left\|\phi^{k+1} - \phi^k\right\|_{L^2}^2 \\ &+ \frac{1}{2}\left(J * \left(\phi^{k+1} - \phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2} \ . \end{aligned} \tag{4.6}$$

Moreover, for any $k \geq 1$,

$$\int_\Omega \phi^k \, d\mathbf{x} = \int_\Omega \phi^0 \, d\mathbf{x}. \tag{4.7}$$

The remainder term, $R_1^c\left(\phi^k, \phi^{k+1}\right)$*, is non-negative, which implies that the energy is non-increasing for any* s, i.e., $E\left(\phi^{k+1}\right) \leq E\left(\phi^k\right)$. *Similarly, if* ϕ^{k+1}, $w^{k+\frac{1}{2}} \in C_p^\infty(\Omega)$ *are pair of solutions to the nCH scheme (4.3) – (4.4). Then for any* $s > 0$,

$$E\left(\phi^{k+1}\right) + s\left\|w^{k+1}\right\|_{L^2}^2 + R_1^c\left(\phi^k, \phi^{k+1}\right) = E\left(\phi^k\right) \ , \tag{4.8}$$

and we say that these two schemes are unconditionally energy stable.

Proof. To prove the conservation of mass for the nCH scheme (4.1) – (4.2) we test Eq. (4.1) with 1, thus for any $k \geq 0$

$$\left(\phi^{k+1} - \phi^k, 1\right)_{L^2} = s\left(\Delta w^{k+1}, 1\right)_{L^2} = -s\left(\nabla w^{k+1}, \nabla 1\right)_{L^2} = 0 \ . \tag{4.9}$$

For Eq. (4.5), we note the following identities. Using $a(a-b)=\frac{1}{2}\left(a^2-b^2+(a-b)^2\right)$, we have

$$\begin{aligned}
& \left(\left(\phi^{k+1}\right)^3, \phi^{k+1}-\phi^k\right)_{L^2} \\
= & \left(\left(\phi^{k+1}\right)^2, \phi^{k+1}\left(\phi^{k+1}-\phi^k\right)\right)_{L^2} \\
= & \left(\left(\phi^{k+1}\right)^2, \frac{\left(\phi^{k+1}\right)^2}{2}-\frac{\left(\phi^k\right)^2}{2}+\frac{1}{2}\left(\phi^{k+1}-\phi^k\right)^2\right)_{L^2} \\
= & \left(1, \frac{\left(\phi^{k+1}\right)^4}{2}-\frac{\left(\phi^{k+1}\phi^k\right)^2}{2}+\frac{1}{2}\left(\phi^{k+1}\right)^2\left(\phi^{k+1}-\phi^k\right)^2\right)_{L^2} \\
= & \frac{1}{4}\left\|\phi^{k+1}\right\|_{L^4}^4-\frac{1}{4}\left\|\phi^k\right\|_{L^4}^4+\frac{1}{4}\left\|\left(\phi^{k+1}\right)^2-\left(\phi^k\right)^2\right\|_{L^2}^2 \\
& +\frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1}-\phi^k\right)\right\|_{L^2}^2 .
\end{aligned} \tag{4.10}$$

Likewise

$$\left(\phi^{k+1}, \phi^{k+1}-\phi^k\right)_{L^2}=\frac{1}{2}\left\|\phi^{k+1}\right\|_{L^2}^2-\frac{1}{2}\left\|\phi^k\right\|_{L^2}^2+\frac{1}{2}\left\|\phi^{k+1}-\phi^k\right\|_{L^2}^2, \tag{4.11}$$

and

$$\left(\phi^k, \phi^{k+1}-\phi^k\right)_{L^2}=\frac{1}{2}\left\|\phi^k\right\|_{L^2}^2-\frac{1}{2}\left\|\phi^{k+1}\right\|_{L^2}^2+\frac{1}{2}\left\|\phi^{k+1}-\phi^k\right\|_{L^2}^2 . \tag{4.12}$$

And, finally,

$$\begin{aligned}
\left(J*\phi^k, \phi^{k+1}-\phi^k\right)_{L^2} = & \frac{1}{2}\left(J*\phi^k, \phi^k\right)_{L^2}-\frac{1}{2}\left(J*\phi^{k+1}, \phi^{k+1}\right)_{L^2} \\
& +\frac{1}{2}\left(J*\left(\phi^{k+1}-\phi^k\right), \phi^{k+1}-\phi^k\right)_{L^2} .
\end{aligned} \tag{4.13}$$

Now, testing Eq. (4.1) with w^{k+1}, we obtain

$$\left(\phi^{k+1}-\phi^k, w^{k+1}\right)_{L^2}=-s\left\|\nabla w^{k+1}\right\|_{L^2}^2, \tag{4.14}$$

where

$$\begin{aligned}\left(\phi^{k+1}-\phi^{k}, w^{k+1}\right)_{L^2} &= \left(\left(\phi^{k+1}\right)^3, \phi^{k+1}-\phi^{k}\right)_{L^2} \\ &\quad + \left(2J_c * 1+\gamma_c\right)\left(\phi^{k+1}, \phi^{k+1}-\phi^{k}\right)_{L^2} \\ &\quad - \left(J_c * 1 + J_e * 1 + \gamma_e\right)\left(\phi^{k}, \phi^{k+1}-\phi^{k}\right)_{L^2} \\ &\quad - \left(J * \phi^{k}, \phi^{k+1}-\phi^{k}\right)_{L^2}. \end{aligned} \tag{4.15}$$

Using identities (4.10) – (4.13) in the last equation, we get

$$\begin{aligned}\left(\phi^{k+1}-\phi^{k}, w^{k+1}\right)_{L^2} &= \frac{1}{4}\left\|\phi^{k+1}\right\|_{L^4}^4 - \frac{1}{4}\left\|\phi^{k}\right\|_{L^4}^4 + \frac{1}{4}\left\|\left(\phi^{k+1}\right)^2-\left(\phi^{k}\right)^2\right\|_{L^2}^2 \\ &\quad + \frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1}-\phi^{k}\right)\right\|_{L^2}^2 \\ &\quad + \frac{2J_c * 1+\gamma_c}{2}\left\|\phi^{k+1}\right\|_{L^2}^2 - \frac{2J_c * 1+\gamma_c}{2}\left\|\phi^{k}\right\|_{L^2}^2 \\ &\quad + \frac{2J_c * 1+\gamma_c}{2}\left\|\phi^{k+1}-\phi^{k}\right\|_{L^2}^2 \\ &\quad - \frac{J_c * 1 + J_e * 1 + \gamma_e}{2}\left\|\phi^{k+1}\right\|_{L^2}^2 \\ &\quad + \frac{J_c * 1 + J_e * 1 + \gamma_e}{2}\left\|\phi^{k}\right\|_{L^2}^2 \\ &\quad + \frac{J_c * 1 + J_e * 1 + \gamma_e}{2}\left\|\phi^{k+1}-\phi^{k}\right\|_{L^2}^2 \\ &\quad - \frac{1}{2}\left(J * \phi^{k+1}, \phi^{k+1}\right)_{L^2} + \frac{1}{2}\left(J * \phi^{k}, \phi^{k}\right)_{L^2} \\ &\quad + \frac{1}{2}\left(J * \left(\phi^{k+1}-\phi^{k}\right), \phi^{k+1}-\phi^{k}\right)_{L^2} \\ &= E\left(\phi^{k+1}\right) - E\left(\phi^{k}\right) \\ &\quad + \frac{1}{4}\left\|\left(\phi^{k+1}\right)^2-\left(\phi^{k}\right)^2\right\|_{L^2}^2 + \frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1}-\phi^{k}\right)\right\|_{L^2}^2 \\ &\quad + \frac{3J_c * 1 + J_e * 1 + \gamma_c + \gamma_e}{2}\left\|\phi^{k+1}-\phi^{k}\right\|_{L^2}^2 \\ &\quad + \frac{1}{2}\left(J * \left(\phi^{k+1}-\phi^{k}\right), \phi^{k+1}-\phi^{k}\right) \\ &= E\left(\phi^{k+1}\right) - E\left(\phi^{k}\right) + R_1^c\left(\phi^{k}, \phi^{k+1}\right) \;. \end{aligned} \tag{4.16}$$

Next, we show that $R_1^c\left(\phi^k, \phi^{k+1}\right) \geq 0$. Clearly

$$
\begin{aligned}
R_1^c\left(\phi^k, \phi^{k+1}\right) & \geq \frac{3J_c * 1 + J_e * 1}{2}\left\|\phi^{k+1} - \phi^k\right\|_{L^2}^2 \\
& \quad + \frac{1}{2}\left(J * \left(\phi^{k+1} - \phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2} \\
& = \frac{3J_c * 1}{2}\left\|\phi^{k+1} - \phi^k\right\|_{L^2}^2 + \frac{J_e * 1}{2}\left\|\phi^{k+1} - \phi^k\right\|_{L^2}^2 \\
& \quad + \frac{1}{2}\left(J_c * \left(\phi^{k+1} - \phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2} \\
& \quad - \frac{1}{2}\left(J_e * \left(\phi^{k+1} - \phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2} \\
& \geq (J_c * 1)\left\|\phi^{k+1} - \phi^k\right\|_{L^2}^2 \ ,
\end{aligned} \tag{4.17}
$$

where we have used Young inequality in the last step. For Eq. (4.8) we test Eq. (4.3) with w^{k+1} and obtain

$$
\left(\phi^{k+1} - \phi^k, w^{k+1}\right)_{L^2} = -s\left\|w^{k+1}\right\|_{L^2}^2 \ , \tag{4.18}
$$

and the rest part of the proof is the same. □

4.3 The Discrete Energy

We begin by defining a fully discrete energy that is consistent with the continuous space energy (1.12). In particular, define the discrete energy $F : \mathcal{C}_{m\times n} \to \mathbb{R}$ to be

$$
F(\phi) := \frac{1}{4}\|\phi\|_4^4 + \frac{\gamma_c - \gamma_e}{2}\|\phi\|_2^2 + \frac{[J \star \mathbf{1}]}{2}\|\phi\|_2^2 - \frac{1}{2}\left(\phi \| [J \star \phi]\right) \ , \tag{4.19}
$$

where $J : \mathbb{R}^2 \to \mathbb{R}$ is a correlation function with properties (J1) – (J3). Here we view J as a function in $\mathcal{V}_{m\times n}$ via the identification $J_{i+\frac{1}{2}, j+\frac{1}{2}} := J(p_{i+\frac{1}{2}}, p_{j+\frac{1}{2}})$. Also we need to define the fully discrete pseudo energy

$$\begin{aligned}\mathcal{F}\left(\phi^k,\phi^{k+1}\right) &:= F\left(\phi^{k+1}\right) + \frac{[J_c \star \mathbf{1}] + [J_e \star \mathbf{1}] + \gamma_e}{4}\left\|\phi^{k+1}-\phi^k\right\|_2^2 \\ &\quad + \frac{h^2}{4}\left(\left[J\star\left(\phi^{k+1}-\phi^k\right)\right]\middle\|\phi^{k+1}-\phi^k\right) \ . \end{aligned} \tag{4.20}$$

where $F(\phi)$ is as defined in Eq. (4.19). We now need a discrete counterparts of Lem. 1.2.1.

Lemma 4.3.1. *Suppose that $\phi \in \mathcal{C}_{m\times n}$ is periodic. There exists a non-negative constant C_0 such that for all $F(\phi) + C_0 \geq 0$. More specifically,*

$$\frac{1}{8}\|\phi\|_4^4 \leq F(\phi) + \frac{\left(\gamma_c - \gamma_e - 2\left[J_e \star \mathbf{1}\right]\right)^2}{2}|\Omega|, \tag{4.21}$$

$$\frac{1}{2}\|\phi\|_2^2 \leq F(\phi) + \frac{\left(\gamma_c - \gamma_e - 2\left[J_e \star \mathbf{1}\right] - 1\right)^2}{2}|\Omega|. \tag{4.22}$$

Moreover, $F(\phi^{k+1}) \leq \mathcal{F}(\phi^k, \phi^{k+1})$.

Proof. By Lem. 3.3.2,

$$\begin{aligned}\frac{[J\star 1]}{2}\|\phi\|_2^2 - \frac{h^2}{2}\left(\phi\|[J\star\phi]\right) &= \frac{[J_c\star 1]}{2}\|\phi\|_2^2 - \frac{h^2}{2}\left(\phi\|[J_c\star\phi]\right) \\ &\quad -\frac{[J_e\star 1]}{2}\|\phi\|_2^2 + \frac{h^2}{2}\left(\phi\|[J_e\star\phi]\right) \\ &\geq -\frac{[J_e\star 1]}{2}\|\phi\|^2 + \frac{h^2}{2}\left(\phi\|[J_e\star\phi]\right) \\ &\geq -\frac{[J_e\star 1]}{2}\|\phi\|_2^2 - \frac{[J_e\star 1]}{2}\|\phi\|_2^2 \\ &= -\left[J_e\star 1\right]\|\phi\|_2^2 \ . \end{aligned} \tag{4.23}$$

Set

$$P(\phi) := \frac{1}{4}(\phi)^4 + \frac{\gamma_c}{2}(\phi)^2 - \frac{\gamma_e}{2}(\phi)^2 \ , \quad Q(\phi) := F(\phi) - [J_e\star 1]\,(\phi)^2 \ , \tag{4.24}$$

so that

$$F(\phi) = (P(\phi)\|1) + \frac{[J\star 1]}{2}\,\|\phi\|_2^2 - \frac{h^2}{2}\,(\phi\|[J\star\phi]\,)\ . \tag{4.25}$$

Using (4.23),

$$F(\phi) \geq (Q(\phi)\|1)\ . \tag{4.26}$$

Utilizing the inequalities

$$\frac{1}{8}\,(\phi)^4 \leq Q(\phi) + \frac{(\gamma_c - \gamma_e - 2\,[J_e\star 1]\,)^2}{2}, \tag{4.27}$$

$$\frac{1}{2}\,(\phi)^2 \leq Q(\phi) + \frac{(\gamma_c - \gamma_e - 2\,[J_e\star 1]\, - 1)^2}{4}\ , \tag{4.28}$$

the estimates follow. □

Lemma 4.3.2. (Existence of a Convex Splitting:) *Suppose that* $\phi \in \mathcal{C}_{m\times n}(\Omega)$, *periodic, suppose*

$$F_c(\phi) := \frac{1}{4}\,\|\phi\|_4^4 + \frac{(2\,[J_c\star 1]\, + \gamma_c)}{2}\,\|\phi\|_2^2\,, \tag{4.29}$$

$$F_e(\phi) := \frac{([J_c\star 1]\, + [J_e\star 1]\, + \gamma_e)}{2}\,\|\phi\|_2^2 + \frac{1}{2}\,(\phi\|[J\star\phi]\,)\,. \tag{4.30}$$

Then F_c *and* F_e *are convex, and the gradients of the respective energies are*

$$\delta_\phi F_c = \phi^3 + (2\,[J_c\star 1]\, + \gamma_c)\,\phi\ ,\quad \delta_\phi F_e = ([J_c\star 1]\, + [J_e\star 1]\, + \gamma_e)\,\phi + [J\star\phi]\ . \tag{4.31}$$

Hence F*, as defined in (4.19), admits the convex splitting* $F = F_c - F_e$*.*

Proof. Suppose that $\psi \in \mathcal{C}_{m\times n}$ is periodic. Calculating the (discrete) variation of F_c shows

$$\left.\frac{dF_c}{ds}(\phi + s\psi)\right|_{s=0} = h^2\,\left(\phi^3 + (2\,[J_c\star 1]\, + \gamma_c)\,\phi\big\|\psi\right)\ , \tag{4.32}$$

and the gradient formula follows. A calculation of the second variation reveals

$$\left.\frac{d^2F_c}{ds^2}(\phi + s\psi)\right|_{s=0} = h^2\,\left(3\phi^2\psi^2 + (2\,[J_c\star 1]\, + \gamma_c)\,\psi^2\big\|\mathbf{1}\right) \geq 0\,, \tag{4.33}$$

which proves that F_c is convex.

For F_e, we begin with the definition

$$\begin{aligned} F_e(\phi) = & \frac{\gamma_e}{2} \|\phi\|_2^2 \\ & + h^2 \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{m} \sum_{l=1}^{n} \left(J^c_{k+\frac{1}{2},l+\frac{1}{2}} \frac{1}{2} \left(\phi_{k,j} + \phi_{i,j}\right)^2 + J^e_{k+\frac{1}{2},l+\frac{1}{2}} \frac{1}{2} \left(\phi_{k,j} - \phi_{i,j}\right)^2 \right) \ , \end{aligned} \tag{4.34}$$

where $J^\alpha_{k+\frac{1}{2},l+\frac{1}{2}} := J_\alpha(x_{k+\frac{1}{2}}, y_{l+\frac{1}{2}})$, $\alpha = c,\, e$. Calculating the variation gives

$$\begin{aligned} \left.\frac{dF_e}{ds}(\phi + s\psi)\right|_{s=0} = & h^2 \left(\gamma_e \phi \| \psi\right) \\ & + 2h^2 \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{m} \sum_{l=1}^{n} J^c_{k+\frac{1}{2},l+\frac{1}{2}} \left(\phi_{k,j} + \phi_{i,j}\right) \left(\psi_{k,j} + \psi_{i,j}\right) \\ & + 2h^2 \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{m} \sum_{l=1}^{n} J^e_{k+\frac{1}{2},l+\frac{1}{2}} \left(\phi_{k,j} - \phi_{i,j}\right) \left(\psi_{k,j} - \psi_{i,j}\right) \ , \end{aligned} \tag{4.35}$$

which yields the gradient. Consider the second variation of the energy:

$$\begin{aligned} \left.\frac{d^2F_e}{ds^2}(\phi + s\psi)\right|_{s=0} = & h^2 \ \left(\gamma_e \psi^2 \middle\| \mathbf{1}\right) \\ & + h^2 \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{m} \sum_{l=1}^{n} J^c_{k+\frac{1}{2},l+\frac{1}{2}} \left(\psi_{k,j} + \psi_{i,j}\right)^2 \\ & + h^2 \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1}^{m} \sum_{l=1}^{n} J^e_{k+\frac{1}{2},l+\frac{1}{2}} \left(\psi_{k,j} - \psi_{i,j}\right)^2 \ . \end{aligned} \tag{4.36}$$

Hence, $\left.\frac{d^2F_e}{ds^2}(\phi + s\psi)\right|_{s=0} \geq 0$, which implies that F_e is convex.

□

4.4 The First-Order (In Time) Fully Discrete Scheme

Based on Lem. 4.3.2, we now describe the fully discrete schemes in detail. Define the cell-centered chemical potential $\tilde{w} \in \mathcal{C}_{m\times n}$ to be

$$\begin{aligned} \tilde{w}\left(\phi^{k+1}, \phi^k\right) &:= \delta_\phi F_c(\phi^{k+1}) - \delta_\phi F_e(\phi^k) \\ &= \left(\phi^{k+1}\right)^3 + \left(2\left[J_c \star 1\right] + \gamma_c\right)\phi^{k+1} \\ &\quad - \left(\left[J_c \star 1\right] + \left[J_e \star 1\right] + \gamma_e\right)\phi^k - \left[J \star \phi^k\right] \ . \end{aligned} \tag{4.37}$$

The scheme for nCH (Eq. (1.2)) is the following: given $\phi^k \in \mathcal{C}_{m\times n}$ periodic, find ϕ^{k+1}, $\tilde{w} \in \mathcal{C}_{m\times n}$ periodic such that

$$\phi^{k+1} - \phi^k = s\Delta_h \tilde{w} \ . \tag{4.38}$$

Similarly the scheme for for nAC (Eq. (1.3)) is: given $\phi^k \in \mathcal{C}_{m\times n}$ periodic, find ϕ^{k+1}, $\tilde{w} \in \mathcal{C}_{m\times n}$ periodic such that

$$\phi^{k+1} - \phi^k = -s\tilde{w} \ . \tag{4.39}$$

Notice that this scheme respects the convex splitting of the discrete energy F. The contribution to the chemical potential corresponding to the convex energy F_c is treated implicitly, the part corresponding to the concave part F_e is treated explicitly.

4.5 Unconditional Unique Solvability for First Order Scheme

We now show how the convexity is translated into solvability for the mass-conserving scheme (4.38) and (4.39). The method established in [39] is used.

Theorem 4.2. *The scheme (4.38) for the nCH equation is discretely mass conservative,* i.e., $h^2\left(\phi^{k+1}-\phi^k\middle\|\mathbf{1}\right)=0$, *and uniquely solvable for any time step-size* $s>0$. *Likely the scheme (4.39) for the nAC equation is uniquely solvable for any time step-size* $s>0$.

Proof. For the unique solvability of scheme (4.38), suppose that ϕ^{k+1}, $\tilde{w}\in\mathcal{C}_{m\times n}$ is a periodic solution pair to scheme (4.38). Then summing Eq. (4.38) and using the periodic boundary conditions for $\tilde{w}$ gives

$$
\begin{aligned}
h^2\left(\phi^{k+1}-\phi^k\middle\|\mathbf{1}\right) &= sh^2\left(\Delta_h\tilde{w}\|\mathbf{1}\right)\\
&= -sh^2\left[D_x\tilde{w}\|D_x\mathbf{1}\right]_{\mathrm{ew}}-sh^2\left[D_y\tilde{w}\|D_y\mathbf{1}\right]_{\mathrm{ns}}=0. \qquad (4.40)
\end{aligned}
$$

Hence $h^2\left(\phi^{k+1}\middle\|\mathbf{1}\right)=h^2\left(\phi^k\middle\|\mathbf{1}\right)$, which clearly is a necessary condition for solvability. Consequently, the set of admissible functions is the hyperplane

$$
\mathcal{A}_1=\left\{\phi\in\mathcal{C}_{m\times n}\;\middle|\;(\phi\|\mathbf{1})=\left(\phi^k\middle\|\mathbf{1}\right)\text{ and }\phi\text{ is periodic}\right\}.
$$

Now, consider the following functional on $\mathcal{A}_1$:

$$
G_1^1(\phi):=\frac{1}{2s}\left\|\phi-\phi^k\right\|_H^2+F_c(\phi)-h^2\left(\phi\middle\|\delta_\phi F_e(\phi^k)\right). \qquad (4.41)
$$

Observe that (see, *e.g.*, [39])

$$
\tilde{w}(\phi,\phi^k)=\delta_\phi\left[F_c(\phi)-h^2\left(\phi\middle\|\delta_\phi F_e(\phi^k)\right)\right], \qquad (4.42)
$$

where δ_ϕ is the discrete variational derivative. By Lem. 4.3.2 the functional F_c is strictly convex. This, together with the properties of the H inner product and norm given in Sec. 3.2, implies that $G_1^1(\phi)$ is strictly convex and coercive over $\mathcal{A}_1$. Therefore, its unique minimizer $\phi^{k+1}\in\mathcal{A}_1$ satisfies the discrete Euler-Lagrange equation

$$
\delta_\phi G_1^1\left(\phi^{k+1}\right)=-\Delta_h^{-1}\left(\frac{\phi^{k+1}-\phi^k}{s}\right)+\tilde{w}+C=0, \qquad (4.43)
$$

where C is a constant. This is equivalent to

$$\phi^{k+1} - \phi^k = s\Delta_h \tilde{w}, \tag{4.44}$$

which is just Eq. (4.38). Thus minimizing the strictly convex functional $G_1^1(\phi)$ over the set of admissible functions , the affine space $\mathcal{A}_1$, is the same as solving the first order convex splitting scheme (4.38).

Regarding to the unique solvability of scheme (4.39), consider the functional

$$G_2^1(\phi) := \frac{1}{2s}\left\|\phi - \phi^k\right\|_2^2 + F_c(\phi) - h^2\left(\phi \middle\| \delta_\phi F_e(\phi^k)\right). \tag{4.45}$$

Then $G_2^1(\phi)$ is strictly convex and coercive over the set of admissible functions

$$\mathcal{A}_2 = \left\{\phi \in \mathcal{C}_{m\times n} \mid \phi \text{ is periodic}\right\}, \tag{4.46}$$

and its unique minimizer $\phi^{k+1} \in \mathcal{A}_2$ satisfies the discrete Euler-Lagrange equation

$$\delta_\phi G_2\left(\phi^{k+1}\right) = \frac{\phi^{k+1} - \phi^k}{s} + \tilde{w} = 0, \tag{4.47}$$

which is equivalent to Eq. (4.39). Thus minimizing the strictly convex functional $G_2^1(\phi)$ over the set of admissible functions $\mathcal{A}_2$ is the same as solving the second-order convex splitting scheme (4.39). This completes the second part of the proof. □

4.6 Unconditional Energy and L^4 Stability for the First Order Scheme

The following is a discrete version of Thm. 4.1.

Theorem 4.3. (Energy Stability:) *Suppose the energy $F(\phi)$ is as defined in Eq. (4.19), assume ϕ^{k+1}, $\phi^k \in \mathcal{C}_{m\times n}$ are periodic and they are solutions to the scheme*

(4.38). *Then for any* $s > 0$

$$F\left(\phi^{k+1}\right) + s\left\|\nabla\tilde{w}^{k+1}\right\|_2^2 + R_h\left(\phi^k, \phi^{k+1}\right) = F\left(\phi^k\right) \ , \tag{4.48}$$

where

$$\begin{aligned} R_h\left(\phi^k, \phi^{k+1}\right) &= \frac{1}{4}\left\|\left(\phi^{k+1}\right)^2 - \left(\phi^k\right)^2\right\|_2^2 + \frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1} - \phi^k\right)\right\|_2^2 \\ &+ \frac{3\left[J_c \star 1\right] + \left[J_e \star 1\right] + \gamma_c + \gamma_e}{2}\left\|\phi^{k+1} - \phi^k\right\|_2^2 \\ &+ \frac{h^2}{2}\left(\left[J \star \left(\phi^{k+1} - \phi^k\right)\right] \middle\| \phi^{k+1} - \phi^k\right) \ . \end{aligned} \tag{4.49}$$

The remainder term, $R_h\left(\phi^k, \phi^{k+1}\right)$*, is non-negative, which implies that the energy is non-increasing for any* s*,* i.e., $F\left(\phi^{k+1}\right) \leq F\left(\phi^k\right)$*. Similarly if* ϕ^{k+1}*,* $\phi^k \in \mathcal{C}_{m\times n}$ *are periodic and they are solutions to the scheme (4.39). Then for any* $s > 0$*,*

$$F\left(\phi^{k+1}\right) + s\left\|\tilde{w}^{k+1}\right\|_2^2 + R_h\left(\phi^k, \phi^{k+1}\right) = F\left(\phi^k\right) \ , \tag{4.50}$$

and we say that these two schemes are unconditionally energy stable.

Proof. For equality (4.48), we note the following identities. Using $a(a-b) = \frac{1}{2}\left(a^2 - b^2 + (a-b)^2\right)$, we have

$$\begin{aligned} & h^2\left(\left(\phi^{k+1}\right)^3 \middle\| \phi^{k+1} - \phi^k\right) \\ = \ & h^2\left(\left(\phi^{k+1}\right)^2 \middle\| \phi^{k+1}\left(\phi^{k+1} - \phi^k\right)\right) \\ = \ & h^2\left(\left(\phi^{k+1}\right)^2 \middle\| \frac{\left(\phi^{k+1}\right)^2}{2} - \frac{\left(\phi^k\right)^2}{2} + \frac{1}{2}\left(\phi^{k+1} - \phi^k\right)^2\right) \\ = \ & h^2\left(1 \middle\| \frac{\left(\phi^{k+1}\right)^4}{2} - \frac{\left(\phi^{k+1}\phi^k\right)^2}{2} + \frac{1}{2}\left(\phi^{k+1}\right)^2\left(\phi^{k+1} - \phi^k\right)^2\right) \\ = \ & \frac{1}{4}\left\|\phi^{k+1}\right\|_4^4 - \frac{1}{4}\left\|\phi^k\right\|_4^4 + \frac{1}{4}\left\|\left(\phi^{k+1}\right)^2 - \left(\phi^k\right)^2\right\|_2^2 \\ & + \frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1} - \phi^k\right)\right\|_2^2 . \end{aligned} \tag{4.51}$$

Likewise

$$h^2\left(\phi^{k+1}\middle\|\phi^{k+1}-\phi^k\right)=\frac{1}{2}\left\|\phi^{k+1}\right\|_2^2-\frac{1}{2}\left\|\phi^k\right\|_2^2+\frac{1}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2, \tag{4.52}$$

and

$$-h^2\left(\phi^k\middle\|\phi^{k+1}-\phi^k\right)=\frac{1}{2}\left\|\phi^k\right\|_2^2-\frac{1}{2}\left\|\phi^{k+1}\right\|_2^2+\frac{1}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2. \tag{4.53}$$

And, finally,

$$\begin{aligned}-h^2\left(\left[J\star\phi^k\right]\middle\|\phi^{k+1}-\phi^k\right) &= \frac{h^2}{2}\left(\left[J\star\phi^k\right]\middle\|\phi^k\right)-\frac{h^2}{2}\left(\left[J\star\phi^{k+1}\right]\middle\|\phi^{k+1}\right)\\ &\quad+\frac{h^2}{2}\left(\left[J\star\left(\phi^{k+1}-\phi^k\right)\right]\middle\|\phi^{k+1}-\phi^k\right).\end{aligned} \tag{4.54}$$

Now, testing Eq. (4.38) with $\tilde{w}^{k+1}$, we obtain

$$h^2\left(\phi^{k+1}-\phi^k\middle\|w^{k+1}\right)=-s\left\|\nabla w^{k+1}\right\|_2^2, \tag{4.55}$$

where

$$\begin{aligned}\left(\phi^{k+1}-\phi^k\middle\|w^{k+1}\right) &= \left(\left(\phi^{k+1}\right)^3\middle\|\phi^{k+1}-\phi^k\right)+\left(2\left[J_c\star 1\right]+\gamma_c\right)\left(\phi^{k+1}\middle\|\phi^{k+1}-\phi^k\right)\\ &\quad-\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)\left(\phi^k\middle\|\phi^{k+1}-\phi^k\right)\\ &\quad-\left(\left[J\star\phi^k\right]\middle\|\phi^{k+1}-\phi^k\right).\end{aligned} \tag{4.56}$$

Using identities (4.51) – (4.54) in the last equation, we get

$$\begin{aligned}
h^2\left(\phi^{k+1}-\phi^k \middle\| w^{k+1}\right) &= \frac{1}{4}\left\|\phi^{k+1}\right\|_4^4-\frac{1}{4}\left\|\phi^k\right\|_4^4+\frac{1}{4}\left\|\left(\phi^{k+1}\right)^2-\left(\phi^k\right)^2\right\|_2^2 \\
&+\frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1}-\phi^k\right)\right\|_2^2 \\
&+\frac{2\left[J_c\star 1\right]\,+\gamma_c}{2}\left\|\phi^{k+1}\right\|_{L^2}^2-\frac{2\left[J_c\star 1\right]\,+\gamma_c}{2}\left\|\phi^k\right\|_2^2 \\
&+\frac{2\left[J_c\star 1\right]\,+\gamma_c}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2 \\
&-\frac{\left[J_c\star 1\right]\,+\left[J_e\star 1\right]\,+\gamma_e}{2}\left\|\phi^{k+1}\right\|_2^2 \\
&+\frac{\left[J_c\star 1\right]\,+\left[J_e\star 1\right]\,+\gamma_e}{2}\left\|\phi^k\right\|_2^2 \\
&+\frac{\left[J_c\star 1\right]\,+\left[J_e\star 1\right]\,+\gamma_e}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2 \\
&-\frac{h^2}{2}\left(J*\phi^{k+1}\middle\|\phi^{k+1}\right)+\frac{h^2}{2}\left(J*\phi^k\middle\|\phi^k\right) \\
&+\frac{h^2}{2}\left(J*\left(\phi^{k+1}-\phi^k\right)\middle\|\phi^{k+1}-\phi^k\right) \\
&= F\left(\phi^{k+1}\right)-F\left(\phi^k\right) \\
&+\frac{1}{4}\left\|\left(\phi^{k+1}\right)^2-\left(\phi^k\right)^2\right\|_2^2+\frac{1}{2}\left\|\phi^{k+1}\left(\phi^{k+1}-\phi^k\right)\right\|_2^2 \\
&+\frac{3\left[J_c\star 1\right]\,+\left[J_e\star 1\right]\,+\gamma_c+\gamma_e}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2 \\
&+\frac{1}{2}\left(\left[J\star\left(\phi^{k+1}-\phi^k\right)\right]\,\middle\|\phi^{k+1}-\phi^k\right)\ . \\
&= F\left(\phi^{k+1}\right)-F\left(\phi^k\right)+R_h\left(\phi^k,\phi^{k+1}\right)\ . \qquad (4.57)
\end{aligned}$$

Next, we show that $R_h\left(\phi^k,\phi^{k+1}\right)\geq 0$. Clearly

$$
\begin{aligned}
R_h\left(\phi^k,\phi^{k+1}\right) &\geq \frac{3\left[J_c\star 1\right]+\left[J_e\star 1\right]}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2 \\
&\quad +\frac{h^2}{2}\left(\left[J\star\left(\phi^{k+1}-\phi^k\right)\right]\left\|\phi^{k+1}-\phi^k\right.\right) \\
&= \frac{3\left[J_c\star 1\right]}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2+\frac{\left[J_e\star 1\right]}{2}\left\|\phi^{k+1}-\phi^k\right\|_2^2 \\
&\quad +\frac{h^2}{2}\left(\left[J_c\star\left(\phi^{k+1}-\phi^k\right)\right]\left\|\phi^{k+1}-\phi^k\right.\right) \\
&\quad -\frac{h^2}{2}\left(\left[J_e\star\left(\phi^{k+1}-\phi^k\right)\right]\left\|\phi^{k+1}-\phi^k\right.\right) \\
&\geq \left(J_c * 1\right)\left\|\phi^{k+1}-\phi^k\right\|_2^2 ,
\end{aligned}
\tag{4.58}
$$

where we have used Lem. 3.3.2, in the last step. The result for scheme (4.39) can be proved in the same way. The theorem is proved. □

Corollary 4.6.1. *Suppose that* $\left\{\phi^{k+1},\mu^{k+\frac{1}{2}}\right\}_{k=1}^{\ell}\in\left[\mathcal{C}_{m\times n}\right]^2$ *are a sequence of periodic solutions pairs of the scheme (4.38) with the starting values* ϕ^0*. Then, for any* $1\leq k\leq\ell$*,*

$$
\frac{1}{8}\left\|\phi^k\right\|_4^4 \leq F\left(\phi^0\right)+\frac{\left(\gamma_c-\gamma_e-2\left[J_e\star\mathbf{1}\right]\right)^2}{2}|\Omega|, \tag{4.59}
$$

$$
\frac{1}{2}\left\|\phi^k\right\|_2^2 \leq F\left(\phi^0\right)+\frac{\left(\gamma_c-\gamma_e-2\left[J_e\star\mathbf{1}\right]-1\right)^2}{4}|\Omega|. \tag{4.60}
$$

Proof. By virtue of the Thm. 4.3, we have the chain of inequalities

$$
F\left(\phi^k\right)\leq F\left(\phi^{k-1}\right)\leq\cdots\leq F\left(\phi^0\right). \tag{4.61}
$$

By Lem. 4.3.1, the result is proved. □

Theorem 4.4. (L^4 Stability:) *Let* $\Phi(x,y)$ *be a sufficiently regular, periodic function on* $\Omega=(0,L_{x_1})\times(0\times L_{x_2})$ *and* $\phi_{i,j}^0:=\Phi(p_i,p_j)$*. Suppose* E *is the continuous energy (1.13) and* F *is the discrete energy (4.19). Let* $\phi_{i,j}^k\in\mathcal{C}_{m\times n}$ *be the* k^{th} *periodic solution,* $1\leq k\leq\ell$*, of the scheme (4.38) with the starting values* ϕ^0*. There exist constants,*

$C_1, \ldots C_3 > 0$, *which are independent of* h *and* s, *such that*

$$\max_{1 \le k \le \ell} \left\| \phi^k \right\|_4 \le C_1. \tag{4.62}$$

$$\max_{1 \le k \le \ell} \left\| \phi^k \right\|_2 \le C_2, \tag{4.63}$$

and

$$\sqrt{s \sum_{k=1}^{\ell} \| \nabla_h \tilde{w}^{k+1} \|_2^2} \le C_3. \tag{4.64}$$

Proof. Since the discrete energy F is consistent with E,

$$F\left(\phi^0\right) \le E\left(\Phi\right) + Ch^2 \le E\left(\Phi\right) + C|\Omega|, \tag{4.65}$$

where $C > 0$ is independent of h. Invoking Cor. 4.6.1 and using a second consistency argument on the discrete convolution $[J_e \star \mathbf{1}]$, for all $1 \le k \le \ell$, we have

$$\begin{aligned} \frac{1}{8} \left\| \phi^k \right\|_4^4 &\le F\left(\phi^0\right) + \frac{\left(\gamma_c - \gamma_e - 2\left[J_e \star \mathbf{1}\right]\right)^2}{2} |\Omega|, \\ &\le E\left(\Phi\right) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right)\right)^2}{2} |\Omega| + C|\Omega|, \end{aligned} \tag{4.66}$$

and

$$\begin{aligned} \frac{1}{2} \left\| \phi^k \right\|_2^2 &\le F\left(\phi^0\right) + \frac{\left(\gamma_c - \gamma_e - 2\left[J_e \star \mathbf{1}\right] - 1\right)^2}{4} |\Omega| \\ &\le E\left(\Phi\right) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right) - 1\right)^2}{4} |\Omega| + C|\Omega|. \end{aligned} \tag{4.67}$$

The right-hand-sides are clearly independent of h and s, and the first two *a priori* bounds are proven. The third and fourth follow by summing the estimates in Thm. 4.3, to yield

$$s \sum_{k=1}^{\ell} \left\| \nabla_h \tilde{w}^{k+1} \right\|_2^2 \le F\left(\phi^0\right) \tag{4.68}$$

and using the consistency arguments as above. □

4.7 Local-in-Time Convergence and L^∞ bound for nCH Equation

We conclude this chapter with a local-in-time error estimate for the nCH equation. With different assumptions we can prove either unconditional or conditional convergence for the error, and we will present both.

The existence and uniqueness of a smooth, periodic solution to the nCH with smooth initial data may be established using techniques developed by P.Bates and J.Han in [6, 7]. In the following pages we denote this PDE solution by Φ. By the result of Bates it is also reasonable to assume that $\|\Phi\|_4 < \infty$, and $\|\Phi\|_\infty, \|D\Phi\|_\infty < \infty$ if $J * 1 + \gamma_c - \gamma_e \geq 0$ for any $t \geq 0$. In the next theorem we establish an error estimate for the fully discrete approximation to Φ.

Theorem 4.5. (First Convergence Theorem:) *Given smooth, periodic initial data $\Phi(x, y, t = 0)$, suppose the unique, smooth, periodic solution for the nCH equation (1.2) is given by $\Phi(x, y, t)$ on Ω for $0 < t \leq T$, for some $T < \infty$. Define $\Phi^k_{i,j} := \Phi(x_i, y_j, ks)$, and $e^k_{i,j} := \Phi^k_{i,j} - \phi^k_{i,j}$, where $\phi^k_{i,j} \in \mathcal{C}_{m\times n}$ is k^{th} periodic solution of (4.38) with $\phi^0_{i,j} := \Phi^0_{i,j}$. Then we have*

$$\left\|e^\ell\right\|_2 \leq C\left(h^2 + s\right),\ \ \ell \cdot s \leq T,\ \ C > 0 \text{ is independent of } h \text{ and } s, \tag{4.69}$$

provided s is sufficiently small, $[J \star 1] + \gamma_c - \gamma_e \geq C_2$ for some positive C_2 sufficiently large and independent of h.

Proof. The continuous function Φ solves the discrete equations

$$\Phi^{k+1} - \Phi^k = s\Delta_h \tilde{w}\left(\Phi^{k+1}, \Phi^k\right) + s\tau^{k+1}\ , \tag{4.70}$$

where τ^{k+1} is the local truncation error, which satisfies

$$\left|\tau^{k+1}_{i,j}\right| \leq M_{12}\left(h^2 + s\right)\ , \tag{4.71}$$

for all i, j, and k for some $M_{12} \geq 0$ that depends only on T, L_{x_1} and L_{x_2}. Subtracting Eq. (4.38) from Eq. (4.70) yields

$$e^{k+1} - e^k = s\Delta_h \left(\tilde{w}\left(\Phi^{k+1}, \Phi^k\right) - \tilde{w}\left(\phi^{k+1}, \phi^k\right)\right) + s\tau^{k+1}. \tag{4.72}$$

Multiplying by $2h^2 e^{k+1}$, summing over i and j, and applying Green's second identity (3.2.3) we have

$$\begin{aligned}
\left\|e^{k+1}\right\|_2^2 - \left\|e^k\right\|_2^2 + \left\|e^{k+1} - e^k\right\|_2^2 &= 2h^2 s\left(\tilde{\mu}\left(\Phi^{k+1}, \Phi^k\right) - \tilde{\mu}\left(\phi^{k+1}, \phi^k\right)\middle\|\Delta_h e^{k+1}\right) \\
&\quad +2h^2 s\left(\tau^{k+1}\middle\|e^{k+1}\right) \\
&= 2h^2 s\left(\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3\middle\|\Delta_h e^{k+1}\right) \\
&\quad +2h^2 s\left(2\left[J_c \star 1\right] + \gamma_c\right)\left(e^{k+1}\middle\|\Delta_h e^{k+1}\right) \\
&\quad -2h^2 s\left(\left[J_c \star 1\right] + \left[J_e \star 1\right] + \gamma_e\right)\left(e^k\middle\|\Delta_h e^{k+1}\right) \\
&\quad -2h^2 s\left(\left[J \star e^k\right]\middle\|\Delta_h e^{k+1}\right) \\
&\quad +2h^2 s\left(\tau^{k+1}\middle\|e^{k+1}\right).
\end{aligned} \tag{4.73}$$

By Lem. 3.4.1,

$$2h^2 s\left(\left(\Phi^{k+1}\right)^3 - \left(\phi^{k+1}\right)^3\middle\|\Delta_h e^{k+1}\right) \leq sM_2\left\|\nabla_h e^{k+1}\right\|_2^2 . \tag{4.74}$$

Using summation-by-parts

$$2h^2 s\left(2\left[J_c \star 1\right] + \gamma_c\right)\left(e^{k+1}\middle\|\Delta_h e^{k+1}\right) = -2s\left(2\left[J_c \star 1\right] + \gamma_c\right)\left\|\nabla_h e^{k+1}\right\|_2^2 . \tag{4.75}$$

By Prop. 3.4.1

$$\begin{aligned}
&-2h^2 s\left(\left[J_c \star 1\right] + \left[J_e \star 1\right] + \gamma_e\right)\left(e^k\middle\|\Delta_h e^{k+1}\right) \\
&\leq s\left(\left[J_c \star 1\right] + \left[J_e \star 1\right] + \gamma_e\right)\left(\left\|\nabla_h e^k\right\|_2^2 + \left\|\nabla_h e^{k+1}\right\|_2^2\right) .
\end{aligned} \tag{4.76}$$

By Lem. 3.4.2

$$-2h^2 s\left(\left[J\star e^k\right]\big\|\Delta_h e^{k+1}\right)\leq sM_{11}\frac{1}{\alpha_2}\left\|e^k\right\|_2^2+s\alpha_2\left\|\nabla_h e^{k+1}\right\|_2^2\ . \tag{4.77}$$

And also

$$2h^2 s\left(\tau^{k+1}\big\|e^{k+1}\right)\ \leq\ sM_{12}\left(h^2+s\right)^2+s\left\|e^{k+1}\right\|_2^2\ . \tag{4.78}$$

Combining the above results, we have

$$\begin{aligned}\left\|e^{k+1}\right\|_2^2-\left\|e^k\right\|_2^2\leq & sM_2\left\|\nabla_h e^{k+1}\right\|_2^2-2s\left(2\left[J_c\star 1\right]+\gamma_c\right)\left\|\nabla_h e^{k+1}\right\|_2^2\\ &+s\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)\left\|\nabla_h e^k\right\|_2^2\\ &+s\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)\left\|\nabla_h e^{k+1}\right\|_2^2\\ &+s\frac{M_{11}}{\alpha_2}\left\|e^k\right\|_2^2+s\alpha_2\left\|\nabla_h e^{k+1}\right\|_2^2+sM_{12}(h^2+s)^2+s\left\|e^{k+1}\right\|_2^2\ .\end{aligned} \tag{4.79}$$

Therefore,

$$\begin{aligned}&\left\|e^{k+1}\right\|_2^2-\left\|e^k\right\|_2^2-s\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)\left(\left\|\nabla_h e^k\right\|_2^2-\left\|\nabla_h e^{k+1}\right\|_2^2\right)\\ \leq & s\left(M_2+\alpha_2+2\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)+1-2\left(2\left[J_c\star 1\right]+\gamma_c\right)\right)\left\|\nabla_h e^{k+1}\right\|_2^2\\ &+sM_7(h^2+s)^2+sM_6\left\|e^k\right\|_2^2+s\left\|e^{k+1}\right\|_2^2\\ \leq & s\left(M_2+\alpha_2-2\left[J\star 1\right]-2\left(\gamma_c-\gamma_e\right)\right)\left\|\nabla_h e^{k+1}\right\|_2^2\\ &+s\frac{M_{11}}{\alpha_2}\left\|e^k\right\|_2^2+sM_{12}(h^2+s)^2+s\left\|e^{k+1}\right\|_2^2\ .\end{aligned} \tag{4.80}$$

Summing over k and using $e^0 = 0$, we have

$$\begin{aligned}
&\left\|e^l\right\|_2^2 - s\left([J_c \star 1] + [J_e \star 1] + \gamma_e\right)\left\|\nabla_h e^0\right\|_2^2 + s\left([J_c \star 1] + [J_e \star 1] + \gamma_e\right)\left\|\nabla_h e^l\right\|_2^2 \\
=&\sum_{k=0}^{l-1}\left\{\left\|e^{k+1}\right\|_2^2 - \left\|e^k\right\|_2^2 - s\left([J_c \star 1] + [J_e \star 1] + \gamma_e\right)\left(\left\|\nabla_h e^k\right\|_2^2 - \left\|\nabla_h e^{k+1}\right\|_2^2\right)\right\} \\
\leq& s\frac{M_{11}}{\alpha_2}\sum_{k=0}^{l-1}\left\|e^k\right\|_2^2 + s\sum_{k=0}^{l-1}\left\|e^{k+1}\right\|_2^2 + sM_{12}\sum_{k=0}^{l-1}(h^2+s)^2 \\
&+ s\left(M_2 + \alpha_2 - 2\left[J \star 1\right] - 2\left(\gamma_c - \gamma_e\right)\right)\sum_{k=0}^{l-1}\left\|\nabla_h e^l\right\|_2^2 \ . \qquad (4.81)
\end{aligned}$$

Thus as long as J satisfies:

$$[J \star 1] + \gamma_c - \gamma_e \geq \frac{M_2 + \alpha_2}{2} \ , \qquad (4.82)$$

the following inequality holds:

$$\left\|e^l\right\|_2^2 \leq s\frac{M_{11}}{\alpha_2}\sum_{k=0}^{l-1}\left\|e^k\right\|_2^2 + s\sum_{k=0}^{l-1}\left\|e^{k+1}\right\|_2^2 + sM_{12}\sum_{k=0}^{l-1}(h^2+s)^2 \ . \qquad (4.83)$$

Furthermore, the above inequality implies:

$$\begin{aligned}
\left\|e^l\right\|_2^2 \leq& s\frac{M_{11}}{\alpha_2}\sum_{k=1}^{l-1}\left\|e^k\right\|_2^2 + s\sum_{k=1}^{l}\left\|e^k\right\|_2^2 + sM_{12}\sum_{k=0}^{l-1}(h^2+s)^2 \\
\leq& s(\frac{M_{11}}{\alpha_2} + 1)\left\|e^l\right\|_2^2 + s\left(\frac{M_{11}}{\alpha_2} + 1\right)\sum_{k=1}^{l-1}\left\|e^k\right\|_2^2 + sM_{12}\sum_{k=0}^{l-1}(h^2+s)^2 \ . \qquad (4.84)
\end{aligned}$$

Thus by setting $s < \frac{1}{\frac{M_{11}}{\alpha_2}+1}$, we arrive at

$$\left\|e^l\right\|_2^2 \leq \frac{s\left(\frac{M_{11}}{\alpha_2} + 1\right)}{1 - \left(\frac{M_{11}}{\alpha_2} + 1\right)s}\sum_{k=1}^{l-1}\left\|e^k\right\|_2^2 + sM_{12}\sum_{k=0}^{l-1}(h^2+s)^2 \ . \qquad (4.85)$$

Denote $ls \leq T$, we have

$$\left\|e^l\right\|_2^2 \leq \frac{s\left(\frac{M_{11}}{\alpha_2}+1\right)}{1-s\left(\frac{M_{11}}{\alpha_2}+1\right)} \sum_{k=1}^{l-1} \left\|e^k\right\|_2^2 + sTM_{12}(h^2+s)^2 \ . \tag{4.86}$$

An application of discrete Gronwall inequality yields

$$\left\|e^l\right\|_2^2 \leq \frac{TM_{12}}{1-s\left(\frac{M_{11}}{\alpha_2}+1\right)} \left(1+\frac{s\left(\frac{M_{11}}{\alpha_2}+1\right)}{1-s\left(\frac{M_{11}}{\alpha_2}+1\right)}\right)^{l-1} (h^2+s)^2 \ . \tag{4.87}$$

□

Corollary 4.7.1. *If the assumption of Thm. 4.5 is satisfied with extra assumption that $s \leq h^2$, then the solution ψ^k of the scheme (4.38) satisfies $\left\|\psi^k\right\|_\infty < \infty$ for any k.*

Proof. By Thm. 4.5 there exists a positive constant C independent of s and h, such that

$$\left\|\Phi^k - \phi^k\right\|_2 \leq C(h^2+s) \ . \tag{4.88}$$

Therefore by the inverse inequality

$$\left\|\Phi^k - \phi^k\right\|_\infty \leq \frac{1}{h}\left\|\Phi^k - \phi^k\right\|_2 \leq C(h+\frac{s}{h}) \ . \tag{4.89}$$

Thus if $s \leq h^2$, $\left\|\Phi^k - \phi^k\right\|_\infty \leq 2Ch$. This with triangle inequality yields:

$$\left\|\phi^k\right\|_\infty \leq \left\|\Phi^k\right\|_\infty + 2Ch \ . \tag{4.90}$$

Since $\left\|\Phi^k\right\|_\infty < \infty$, the result followed. □

Remark 4.7.1. *In the first convergence theorem (Thm. 4.5) the size of time step s is independent of the grid size h. However, there exists a lower bound for $[J \star 1]$ and this lower bound is potentially large. We will present the second convergence theorem* *which loose the constraints for the lower bound of* $[J \star 1]$*. In trade-off, the upper bound of* s *in the second convergence theorem has the dependency on* h*.*

Theorem 4.6. (Second Convergence Theorem:) *Given smooth, periodic initial data* $\Phi(x, y, t = 0)$*, suppose the unique, smooth, periodic solution for the nCH equation (1.2) is given by* $\Phi(x, y, t)$ *on* Ω *for* $0 < t \leq T$*, for some* $T < \infty$*. Define* $\Phi_{i,j}^k := \Phi(x_i, y_j, ks)$*, and* $e_{i,j}^k := \Phi_{i,j}^k - \phi_{i,j}^k$*, where* $\phi_{i,j}^k \in \mathcal{C}_{m\times n}$ *is* k^{th} *periodic solution of Eq. (4.38) with* $\phi_{i,j}^0 := \Phi_{i,j}^0$*. Then we have*

$$\left\|e^\ell\right\|_2 \leq C\left(h^2 + s\right), \ \ell \cdot s \leq T, \ C > 0 \text{ is independent of } h \text{ and } s, \tag{4.91}$$

provided s *is sufficiently small and* $s \leq h^2$*,* $[J \star 1] + \gamma_c - \gamma_e > 0$*. Moreover,* $\left\|\phi^k\right\|_\infty < \infty$*.*

Proof. The continuous function Φ solves the discrete equations

$$\Phi^{k+1} - \Phi^k = s\Delta_h \tilde{w}\left(\Phi^{k+1}, \Phi^k\right) + s\tau^{k+1} \ . \tag{4.92}$$

The local truncation error τ^{k+1} satisfies

$$\left|\tau_{i,j}^{k+1}\right| \leq M_{12}\left(h^2 + s\right) \ , \tag{4.93}$$

for all i, j, and k for some $M_{12} \geq 0$ that depends only on T, L_{x_1} and L_{x_2}. By using the cut-off function defined as Eq. (2.41), one can create a new nCH type system:

$$\begin{aligned} \widehat{\Phi}_t =& \Delta w\left(\widehat{\Phi}\right) \ , \\ w\left(\widehat{\Phi}\right) =& F_{M_3}\left(\widehat{\Phi}\right) + \left(\gamma_c - \gamma_e\right)\widehat{\Phi} + (J * 1)\widehat{\Phi} - J * \widehat{\Phi} \ . \end{aligned} \tag{4.94}$$

Notice that by denoting $M_3 < 2\left(1 + \|\Phi\|_\infty\right) < \infty$, Eq. (4.94) and Eq. (1.2) is indeed equivalent, thus $\Phi = \widehat{\Phi}$. This shows that

$$\widehat{\Phi}^{k+1} - \widehat{\Phi}^{k} = s\Delta_h \tilde{w}\left(\widehat{\Phi}^{k+1}, \widehat{\Phi}^{k}\right) + s\tau^{k+1} \ . \tag{4.95}$$

To this new nCH type system we can also derive the corresponding convex splitting scheme:

$$\begin{aligned} \widehat{\phi}^{k+1} - \widehat{\phi}^{k} =& s\Delta\tilde{w} \ , \\ \tilde{w} =& F_{M_3}\left(\widehat{\phi}^{k+1}\right) + \left(2\left[J_c \star 1\right] + \gamma_c\right)\widehat{\phi}^{k+1} \\ & - \left(\left[J_c \star 1\right] + \left[J_e \star 1\right] + \gamma_e\right)\widehat{\phi}^{k} - \left[J \star \widehat{\phi}^{k}\right] \ . \end{aligned} \tag{4.96}$$

Subtracting Eq. (4.96) from Eq. (4.95),

$$\widehat{e}^{k+1} - \widehat{e}^{k} = s\Delta\left(\tilde{w}\left(\widehat{\Phi}^{k+1}, \widehat{\Phi}^{k}\right) - \tilde{w}\left(\widehat{\phi}^{k+1}, \widehat{\phi}^{k}\right)\right) + s\tau^{k+1} \ , \tag{4.97}$$

where $\widehat{e}^{k}$ is defined as

$$\widehat{e}^{k} = \widehat{\Phi}^{k} - \widehat{\phi}^{k} \ . \tag{4.98}$$

Multiplying both sides by $2h^2\widehat{e}^{k+1}$, summing over i and j, applying summation-by-parts, we have

$$\begin{aligned} \left\|\widehat{e}^{k+1}\right\|_2^2 - \left\|\widehat{e}^{k}\right\|_2^2 + \left\|\widehat{e}^{k+1} - \widehat{e}^{k}\right\|_2^2 =& 2h^2 s\left(\tilde{w}\left(\widehat{\Phi}^{k+1}, \widehat{\Phi}^{k}\right) - \tilde{w}\left(\widehat{\phi}^{k+1}, \widehat{\phi}^{k}\right)\middle\| \Delta_h\widehat{e}^{k+1}\right) \\ & + 2h^2 s\left(\tau^{k+1}\middle\|\widehat{e}^{k+1}\right) \\ =& 2h^2 s\left(F_{M_3}\left(\widehat{\Phi}\right) - F_{M_3}\left(\widehat{\phi}\right)\middle\|\Delta_h\widehat{e}^{k+1}\right) \\ & + 2h^2 s\left(2\left[J_c \star 1\right] + \gamma_c\right)\left(\widehat{e}^{k+1}\middle\|\Delta_h\widehat{e}^{k+1}\right) \\ & - 2h^2 s\left(\left[J_c \star 1\right] + \left[J_e \star 1\right] + \gamma_e\right)\left(\widehat{e}^{k}\middle\|\Delta_h\widehat{e}^{k+1}\right) \\ & - 2h^2 s\left(\left[J \star \widehat{e}^{k}\right]\middle\|\Delta_h\widehat{e}^{k+1}\right) \\ & + 2h^2 s\left(\tau^{k+1}\middle\|\widehat{e}^{k+1}\right) \ . \end{aligned}$$

By Lem. 3.5.1,

$$2h^2 s\left(F_{M_3}\left(\widehat{\Phi}\right)-F_{M_3}\left(\widehat{\phi}\right)\middle\|\Delta_h\widehat{e}^{k+1}\right)\leq s\frac{M_7}{\alpha_1}\left\|\widehat{e}^{k+1}\right\|_2^2+\alpha_1 M_8 s\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2+s\frac{M_9}{\alpha_1}h^4\ . \tag{4.99}$$

Using summation-by-parts

$$2h^2 s\left(2\left[J_c\star 1\right]+\gamma_c\right)\left(\widehat{e}^{k+1}\middle\|\Delta_h\widehat{e}^{k+1}\right)=-2s\left(2\left[J_c\star 1\right]+\gamma_c\right)\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\ . \tag{4.100}$$

By Prop. 3.4.1

$$\begin{aligned}&-2h^2 s\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)\left(\widehat{e}^{k}\middle\|\Delta_h\widehat{e}^{k+1}\right)\\ \leq& s\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)\left(\left\|\nabla_h\widehat{e}^{k}\right\|_2^2+\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\right)\ .\end{aligned} \tag{4.101}$$

By Lem. 3.4.2

$$-2h^2 s\left(\left[J\star\widehat{e}^{k}\right]\middle\|\Delta_h\widehat{e}^{k+1}\right)\leq sM_{11}\frac{1}{\alpha_2}\left\|\widehat{e}^{k}\right\|_2^2+s\alpha_2\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\ . \tag{4.102}$$

Meanwhile, we see that

$$2h^2 s\left(\tau^{k+1}\middle\|\widehat{e}^{k+1}\right)\ \leq\ sM_{12}\left(h^2+s\right)^2+s\left\|\widehat{e}^{k+1}\right\|_2^2\ . \tag{4.103}$$

Combining the above results, we have

$$\begin{aligned}\left\|\widehat{e}^{k+1}\right\|_2^2-\left\|\widehat{e}^{k}\right\|_2^2\leq& s\frac{M_7}{\alpha_1}\left\|\widehat{e}^{k+1}\right\|_2^2+\alpha_1 M_8 s\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2+s\frac{M_9}{\alpha_1}h^4\\ &-2s\left(2\left[J_c\star 1\right]+\gamma_c\right)\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\\ &+s\left(\left[J_c\star 1\right]+\left[J_e\star 1\right]+\gamma_e\right)\left(\left\|\nabla_h\widehat{e}^{k}\right\|_2^2+\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\right)\\ &+sM_{11}\frac{1}{\alpha_2}\left\|\widehat{e}^{k}\right\|_2^2+s\alpha_2\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2+sM_{12}(h^2+s)^2+s\left\|\widehat{e}^{k+1}\right\|_2^2\ .\end{aligned} \tag{4.104}$$

This implies

$$
\begin{aligned}
&\left\|\widehat{e}^{k+1}\right\|_2^2-\left\|\widehat{e}^{k}\right\|_2^2-s\left([J_c\star 1]\,+[J_e\star 1]\,+\gamma_e\right)\left(\left\|\nabla_h\widehat{e}^{k}\right\|_2^2-\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\right)\\
\leq& s\left(\alpha_1M_8+\alpha_2-2\left[J\star 1\right]\,-2\left(\gamma_c-\gamma_e\right)\right)\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\\
&+sM_{12}(h^2+s)^2+s\frac{M_9}{\alpha_1}h^4+s\frac{M_{11}}{\alpha_2}\left\|\widehat{e}^{k}\right\|_2^2+s\left(\frac{M_7}{\alpha_1}+1\right)\left\|\widehat{e}^{k+1}\right\|_2^2\\
\leq& s\left(\alpha_1M_8+\alpha_2-2\left[J\star 1\right]\,-2\left(\gamma_c-\gamma_e\right)\right)\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\\
&+s\left(M_{12}+\frac{M_9}{\alpha_1}\right)(h^2+s)^2+s\frac{M_{11}}{\alpha_2}\left\|\widehat{e}^{k}\right\|_2^2+s\left(\frac{M_7}{\alpha_1}+1\right)\left\|\widehat{e}^{k+1}\right\|_2^2\ . \qquad (4.105)
\end{aligned}
$$

Summing over k and using $\widehat{e}^0=0$,

$$
\begin{aligned}
&\left\|\widehat{e}^{l}\right\|_2^2-s\left([J_c\star 1]\,+[J_e\star 1]\,+\gamma_e\right)\left(\left\|\nabla_h\widehat{e}^{0}\right\|_2^2-\left\|\nabla_h\widehat{e}^{l}\right\|_2^2\right)\\
=&\sum_{k=0}^{l-1}\left\{\left\|\widehat{e}^{k+1}\right\|_2^2-\left\|\widehat{e}^{k}\right\|_2^2-s\left([J_c\star 1]\,+[J_e\star 1]\,+\gamma_e\right)\left(\left\|\nabla_h\widehat{e}^{k}\right\|_2^2-\left\|\nabla_h\widehat{e}^{k+1}\right\|_2^2\right)\right\}\\
\leq& s\frac{M_{11}}{\alpha_2}\sum_{k=0}^{l-1}\left\|\widehat{e}^{k}\right\|_2^2+s\left(\frac{M_7}{\alpha_1}+1\right)\sum_{k=0}^{l-1}\left\|\widehat{e}^{k+1}\right\|_2^2+s\left(M_{12}+\frac{M_9}{\alpha_1}\right)\sum_{k=0}^{l-1}(h^2+s)^2\\
&+s\left(\alpha_1M_8+\alpha_2-2\left[J\star 1\right]\,-2\left(\gamma_c-\gamma_e\right)\right)\sum_{k=0}^{l-1}\left\|\nabla_h\widehat{e}^{l}\right\|_2^2\ . \qquad (4.106)
\end{aligned}
$$

Thus if $[J\star 1]\,+\gamma_c-\gamma_e>0$, there exist positive constant α_1 and α_2, such that

$$
[J\star 1]\,+\gamma_c-\gamma_e\geq\frac{\alpha_1M_8+\alpha_2}{2}\ . \qquad (4.107)
$$

Hence the following inequality holds:

$$
\left\|\widehat{e}^{l}\right\|_2^2\leq s\frac{M_{11}}{\alpha_2}\sum_{k=0}^{l-1}\left\|\widehat{e}^{k}\right\|_2^2+s\left(\frac{M_7}{\alpha_1}+1\right)\sum_{k=0}^{l-1}\left\|\widehat{e}^{k+1}\right\|_2^2+s\left(M_{12}+\frac{M_9}{\alpha_1}\right)\sum_{k=0}^{l-1}(h^2+s)^2\ . \qquad (4.108)
$$

Therefore

$$\begin{aligned}\left\|\widehat{e}^{l}\right\|_{2}^{2} \leq & s\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right)\left\|\widehat{e}^{l}\right\|_{2}^{2}+s(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1) \sum_{k=1}^{l-1}\left\|\widehat{e}^{k}\right\|_{2}^{2} \\ & +s\left(M_{12}+\frac{M_{9}}{\alpha_{1}}\right) \sum_{k=0}^{l-1}(h^{2}+s)^{2} \ . \end{aligned} \tag{4.109}$$

The following estimate is valid provided $s < \frac{1}{\frac{M_{11}}{\alpha_2}+\frac{M_7}{\alpha_1}+1}$

$$\left\|\widehat{e}^{l}\right\|_{2}^{2} \leq \frac{s\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right)}{1-\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right) s} \sum_{k=1}^{l-1}\left\|\widehat{e}^{k}\right\|_{2}^{2}+s\left(M_{12}+\frac{M_{9}}{\alpha_{1}}\right) \sum_{k=0}^{l-1}(h^{2}+s)^{2} \ . \tag{4.110}$$

Denote $ls \leq T$,

$$\left\|\widehat{e}^{l}\right\|_{2}^{2} \leq \frac{s\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right)}{1-s\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right)} \sum_{k=1}^{l-1}\left\|\widehat{e}^{k}\right\|_{2}^{2}+sT\left(M_{12}+\frac{M_{9}}{\alpha_{1}}\right)(h^{2}+s)^{2} \ . \tag{4.111}$$

An application of discrete Gronwall inequality yields

$$\left\|\widehat{e}^{l}\right\|_{2}^{2} \leq \frac{T\left(M_{12}+\frac{M_{9}}{\alpha_{1}}\right)}{1-s\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right)}\left(1+\frac{s\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right)}{1-s\left(\frac{M_{11}}{\alpha_{2}}+\frac{M_{7}}{\alpha_{1}}+1\right)}\right)^{l-1}(h^{2}+s)^{2} \ . \tag{4.112}$$

Thus

$$\left\|\widehat{e}^{l}\right\|_{2} \leq C(h^{2}+s) \ . \tag{4.113}$$

Furthermore, by the inverse inequality

$$\left\|\widehat{e}^{l}\right\|_{\infty} \leq \frac{1}{h}\left\|\widehat{e}^{l}\right\|_{2} \ . \tag{4.114}$$

Thus if $s \le h^2$,

$$\left\|\hat{e}^l\right\|_\infty \le 2Ch \ . \tag{4.115}$$

This implies

$$\left\|\hat{\phi}^l\right\|_\infty \le \left\|\hat{\Phi}^l\right\|_\infty + \left\|\hat{e}^l\right\|_\infty \le \left\|\hat{\Phi}^l\right\|_\infty + 2Ch \ . \tag{4.116}$$

Therefore there exist h_0, such that for any $h \le h_0$,

$$\left\|\hat{\phi}^l\right\|_\infty \le M_3 \ . \tag{4.117}$$

Thus $\hat{\phi} = \phi$ and $\hat{e} = e$. □

Chapter 5

Second Order (In Time) Schemes and Their Properties

5.1 Overview

Our principal goal in this section is to describe fully discrete, second order in time, second order in space convex splitting schemes for nCH and nAC equations. We will present the another part of our main results in this chapter: the unconditional solvability of the scheme; the unconditional energy stability and the convergence of the scheme for nAC equation. Due to the difficulty in estimating the second order approximation for the nonlinear term currently we are only be able to show the proof for the convergence of scheme of nAC equation, but numerical evidence presented in Chap. 6 indicates that the scheme of nCH equation has the same convergence property.

The chapter will be organized in following way: in Sec. 5.2 we present the second order in time, continuous in space scheme as the motivation, the energy decreascing property will also be discussed; in Sec. 5.3 we form the fully discrete first order scheme; in Sec. 5.4 we prove the unconditional unique solvability; in Sec. 5.5 we prove the unconditional energy stability and L^p stability; in Sec. 5.6 the convergence of the scheme for nAC will be discussed.

5.2 The Second-Order (In Time) Convex Splitting Scheme

We will use the following function in the rest of the paper:

$$\chi(\phi,\psi) := \frac{1}{2}\left(\phi^2+\psi^2\right). \tag{5.1}$$

A second-order (in time) convex splitting scheme for the nAC equation (1.3) can be constructed as follows: given ϕ^{k-1}, $\phi^k \in C_p^\infty(\Omega)$, find ϕ^{k+1}, $w^{k+\frac{1}{2}} \in C_p^\infty(\Omega)$ such that

$$\phi^{k+1}-\phi^k = -w^{k+\frac{1}{2}}\ , \tag{5.2}$$

$$\begin{aligned} w^{k+\frac{1}{2}} &= \phi^{k+\frac{1}{2}}\chi(\phi^k,\phi^{k+1}) + \left[2(J_c*1)+\gamma_c\right]\phi^{k+\frac{1}{2}} \\ &\quad -\left[(J_c*1)+(J_e*1)+\gamma_e\right]\hat{\phi}^{k+\frac{1}{2}} - J*\hat{\phi}^{k+\frac{1}{2}}\ , \end{aligned} \tag{5.3}$$

where

$$\phi^{k+\frac{1}{2}} := \frac{1}{2}\left(\phi^{k+1}+\phi^k\right)\ ,\quad \hat{\phi}^{k+\frac{1}{2}} := \frac{1}{2}\left(3\phi^k-\phi^{k-1}\right) \tag{5.4}$$

and $\phi^{-1}\equiv\phi^0$. Notice that this scheme respects the convex splitting of the energy E. The contribution to the chemical potential corresponding to the convex energy E_c is treated implicitly, using a second-order secant approximation. The part corresponding to the concave part E_e is treated explicitly, via extrapolation. A second-order convex splitting scheme for the nCH equation (1.2) can be constructed similarly: given

ϕ^{k-1}, $\phi^k \in C_p^\infty(\Omega)$, find ϕ^{k+1}, $w^{k+\frac{1}{2}} \in C_p^\infty(\Omega)$ such that

$$\phi^{k+1} - \phi^k = s\Delta w^{k+\frac{1}{2}} , \tag{5.5}$$

$$\begin{aligned} w^{k+\frac{1}{2}} &= \phi^{k+\frac{1}{2}}\chi(\phi^k, \phi^{k+1}) + \left[2(J_c * 1) + \gamma_c\right]\phi^{k+\frac{1}{2}} \\ &\quad - \left[(J_c * 1) + (J_e * 1) + \gamma_e\right]\hat{\phi}^{k+\frac{1}{2}} - J * \hat{\phi}^{k+\frac{1}{2}} , \end{aligned} \tag{5.6}$$

where $\phi^{-1} \equiv \phi^0$. We need to define a pseudo energy, which we do as follows:

$$\begin{aligned} \mathcal{E}\left(\phi^k, \phi^{k+1}\right) &:= E\left(\phi^{k+1}\right) + \frac{J_c * 1 + J_e * 1 + \gamma_e}{4}\left\|\phi^{k+1} - u^k\right\|_{L^2}^2 \\ &\quad + \frac{1}{4}\left(J * \left(\phi^{k+1} - \phi^k\right), \phi^{k+1} - \phi^k\right)_{L^2} , \end{aligned} \tag{5.7}$$

where $E(\phi)$ is as defined in Eq. (1.12). We can prove the following:

Theorem 5.1. *Suppose the pseudo energy $\mathcal{E}$ is defined as Eq. (5.7). ϕ^{k+1}, $w^{k+\frac{1}{2}} \in C_p^\infty(\Omega)$ is a periodic solution pair to Eq. (5.5) – (5.6). Then, for any $s > 0$,*

$$\mathcal{E}\left(\phi^k, \phi^{k+1}\right) + s\left\|\nabla_h w^{k+\frac{1}{2}}\right\|_{L^2}^2 + R_2^c\left(\phi^{k-1}, \phi^k, \phi^{k+1}\right) = \mathcal{E}\left(\phi^{k-1}, \phi^k\right) , \tag{5.8}$$

where

$$\begin{aligned} R_2^c\left(\phi^{k-1}, \phi^k, \phi^{k+1}\right) &= \frac{J_c * 1 + J_e * 1 + \gamma_e}{4}\left\|\phi^{k+1} - 2\phi^k + \phi^{k-1}\right\|_{L^2}^2 \\ &\quad + \frac{1}{4}\left(J * \left(\phi^{k+1} - 2\phi^k + \phi^{k-1}\right), \phi^{k+1} - 2\phi^k + \phi^{k-1}\right). \end{aligned} \tag{5.9}$$

The remainder term, $R_2^c\left(\phi^{k-1}, \phi^k, \phi^{k+1}\right)$, is non-negative, which implies that the psuedo energy is non-increasing, i.e., $\mathcal{E}\left(\phi^k, \phi^{k+1}\right) \leq \mathcal{E}\left(\phi^{k-1}, \phi^k\right)$. *Similarly, if ϕ^{k+1}, $w^{k+\frac{1}{2}} \in C_p^\infty(\Omega)$ is a periodic solution pair to the scheme (5.2) – (5.3), then, for any $s > 0$,*

$$\mathcal{E}\left(\phi^k, \phi^{k+1}\right) + s\left\|w^{k+\frac{1}{2}}\right\|_2^2 + R\left(\phi^{k-1}, \phi^k, \phi^{k+1}\right) = \mathcal{E}\left(\phi^{k-1}, \phi^k\right) , \tag{5.10}$$

which implies that the pseudo energy is non-increasing, i.e.,

$$\mathcal{E}\left(\phi^k,\phi^{k+1}\right)\le\mathcal{E}\left(\phi^{k-1},\phi^k\right).$$

Proof. We first note the following identities:

$$\left(\phi^{k+\frac{1}{2}}\chi\left(\phi^k,\phi^{k+1}\right),\phi^{k+1}-\phi^k\right)_{L^2}=\frac{1}{4}\left\|\phi^{k+1}\right\|_{L^4}^4-\frac{1}{4}\left\|\phi^k\right\|_{L^4}^4, \tag{5.11}$$

$$\left(\phi^{k+\frac{1}{2}},\phi^{k+1}-\phi^k\right)_{L^2}=\frac{1}{2}\left\|\phi^{k+1}\right\|_{L^2}^2-\frac{1}{2}\left\|\phi^k\right\|_{L^2}^2, \tag{5.12}$$

$$\begin{aligned}\left(\hat{\phi}^{k+\frac{1}{2}},\phi^{k+1}-\phi^k\right)_{L^2} &= -\frac{1}{2}\left\|\phi^{k+1}\right\|_{L^2}^2+\frac{1}{4}\left\|\phi^{k+1}-\phi^k\right\|_{L^2}^2\\ &+\frac{1}{2}\left\|\phi^k\right\|_{L^2}^2-\frac{1}{4}\left\|\phi^k-\phi^{k-1}\right\|_{L^2}^2\\ &+\frac{1}{4}\left\|\phi^{k+1}-2\phi^k+\phi^{k-1}\right\|_{L^2}^2,\end{aligned} \tag{5.13}$$

and

$$\begin{aligned}-\left(J*\hat{\phi}^{k+\frac{1}{2}},\phi^{k+1}-\phi^k\right)_{L^2} &= -\frac{1}{2}\left(J*\phi^{k+1},\phi^{k+1}\right)_{L^2}\\ &+\frac{1}{4}\left(J*\left(\phi^{k+1}-\phi^k\right),\phi^{k+1}-\phi^k\right)_{L^2}\\ &+\frac{1}{2}\left(J*\phi^k,\phi^k\right)_{L^2}-\frac{1}{4}\left(J\left(\phi^k-\phi^{k-1}\right),\phi^k-\phi^{k-1}\right)_{L^2}\\ &+\frac{1}{4}\left(J\left(\phi^{k+1}-2\phi^k+\phi^{k-1}\right),\phi^{k+1}-2\phi^k+\phi^{k-1}\right)_{L^2}\end{aligned} \tag{5.14}$$

Now, testing Eq. (5.5) with $w^{k+\frac{1}{2}}$, we obtain

$$\left(\phi^{k+1}-\phi^k,w^{k+\frac{1}{2}}\right)_{L^2}=-s\left\|\nabla w^{k+\frac{1}{2}}\right\|_{L^2}^2, \tag{5.15}$$

but, considering Eq. (5.6), we have

$$\begin{aligned}\left(\phi^{k+1}-\phi^{k},w^{k+\frac{1}{2}}\right)_{L^2} &= \left(\phi^{k+\frac{1}{2}}\chi\left(\phi^{k},\phi^{k+1}\right),\phi^{k+1}-\phi^{k}\right)_{L^2}\\ &+\left(2J_c*1+\gamma_c\right)\left(\phi^{k+\frac{1}{2}},\phi^{k+1}-\phi^{k}\right)_{L^2}\\ &-\left(J_c*1+J_e*1+\gamma_e\right)\left(\hat{\phi}^{k+\frac{1}{2}},\phi^{k+1}-\phi^{k}\right)_{L^2}\\ &-\left(J*\hat{\phi}^{k+\frac{1}{2}},\phi^{k+1}-\phi^{k}\right)_{L^2}\ . \end{aligned} \tag{5.16}$$

Using identities (5.11) – (5.14) in the last equation, we get

$$\begin{aligned}\left(\phi^{k+1}-\phi^{k},w^{k+1}\right)_{L^2} &= \frac{1}{4}\left\|\phi^{k+1}\right\|_{L^4}^4-\frac{1}{4}\left\|\phi^{k}\right\|_{L^4}^4\\ &+\frac{2J_c*1+\gamma_c}{2}\left\|\phi^{k+1}\right\|_{L^2}^2-\frac{2J_c*\mathbf{1}+\gamma_c}{2}\left\|\phi^{k}\right\|_{L^2}^2\\ &-\frac{J_c*\mathbf{1}+J_e*\mathbf{1}+\gamma_e}{2}\left\|\phi^{k+1}\right\|_{L^2}^2\\ &+\frac{J_c*\mathbf{1}+J_e*\mathbf{1}+\gamma_e}{4}\left\|\phi^{k+1}-\phi^{k}\right\|_{L^2}^2\\ &+\frac{J_c*\mathbf{1}+J_e*\mathbf{1}+\gamma_e}{2}\left\|\phi^{k}\right\|_{L^2}^2\\ &-\frac{J_c*\mathbf{1}+J_e*\mathbf{1}+\gamma_e}{4}\left\|\phi^{k}-\phi^{k-1}\right\|_{L^2}^2\\ &+\frac{J_c*\mathbf{1}+J_e*\mathbf{1}+\gamma_e}{4}\left\|\phi^{k+1}-2\phi^{k}+\phi^{k-1}\right\|_{L^2}^2\\ &-\frac{1}{2}\left(J*\phi^{k+1},\phi^{k+1}\right)_{L^2}+\frac{1}{4}\left(J*\left(\phi^{k+1}-\phi^{k}\right),\phi^{k+1}-\phi^{k}\right)_{L^2}\\ &+\frac{1}{2}\left(J*\phi^{k},\phi^{k}\right)_{L^2}-\frac{1}{4}\left(J*\left(\phi^{k}-\phi^{k-1}\right),\phi^{k}-\phi^{k-1}\right)_{L^2}\\ &+\frac{1}{4}\left(J*\left(\phi^{k+1}-2\phi^{k}+\phi^{k-1}\right),\phi^{k+1}-2\phi^{k}+\phi^{k-1}\right)_{L^2}\\ &= \mathcal{E}\left(\phi^{k},\phi^{k+1}\right)-\mathcal{E}\left(\phi^{k-1},\phi^{k}\right)+R_2^c\left(\phi^{k-1},\phi^{k},\phi^{k+1}\right). \end{aligned} \tag{5.17}$$

The only remaining piece to show is that $R\left(\phi^{k-1},\phi^{k},\phi^{k+1}\right)\geq 0$. But, by Young inequality and the definition of $R\left(\phi^{k-1},\phi^{k},\phi^{k+1}\right)$, this fact is straightforward. The first result is proven. For the second part we testing Eq. (5.2) with $w^{k+\frac{1}{2}}$, we obtain

$$\left(\phi^{k+1}-\phi^{k},w^{k+\frac{1}{2}}\right)_{L^2}=-s\left\|w^{k+\frac{1}{2}}\right\|_{L^2}^2, \tag{5.18}$$

the rest part of the proof is quite similar and is omitted for the sake of brevity. □

5.3 The Second-Order (In Time) Fully Discrete Scheme

A fully second-order convex splitting scheme for the nCH equation can be constructed as follows: given $\phi^k \in \mathcal{C}_{m\times n}$ periodic, find ϕ^{k+1}, $w^{k+\frac{1}{2}} \in \mathcal{C}_{m\times n}$ periodic such that

$$\begin{aligned} \phi^{k+1} - \phi^k &= s\Delta_h w^{k+\frac{1}{2}}, \qquad (5.19) \\ w^{k+\frac{1}{2}} &= \phi^{k+\frac{1}{2}}\chi(\phi^k, \phi^{k+1}) + \left(2\left[J_c \star \mathbf{1}\right] + \gamma_c\right)\phi^{k+\frac{1}{2}} \\ &\quad - \left(\left[J_c \star \mathbf{1}\right] + \left[J_e \star \mathbf{1}\right] + \gamma_e\right)\hat{\phi}^{k+\frac{1}{2}} - \left[J \star \hat{\phi}^{k+\frac{1}{2}}\right], \qquad (5.20) \end{aligned}$$

where

$$\phi^{k+\frac{1}{2}} := \frac{1}{2}\left(\phi^{k+1} + \phi^k\right) \ , \quad \hat{\phi}^{k+\frac{1}{2}} := \frac{1}{2}\left(3\phi^k - \phi^{k-1}\right), \qquad (5.21)$$

and $\phi^{-1} \equiv \phi^0$.

A fully second-order convex splitting scheme for the nAC equation can be constructed as follows: given $\phi^k \in \mathcal{C}_{m\times n}$ periodic, find ϕ^{k+1}, $w^{k+\frac{1}{2}} \in \mathcal{C}_{m\times n}$ periodic such that

$$\begin{aligned} \phi^{k+1} - \phi^k &= -s w^{k+\frac{1}{2}}, \qquad (5.22) \\ w^{k+\frac{1}{2}} &= \phi^{k+\frac{1}{2}}\chi(\phi^k, \phi^{k+1}) + \left(2\left[J_c \star \mathbf{1}\right] + \gamma_c\right)\phi^{k+\frac{1}{2}} \\ &\quad - \left(\left[J_c \star \mathbf{1}\right] + \left[J_e \star \mathbf{1}\right] + \gamma_e\right)\hat{\phi}^{k+\frac{1}{2}} - \left[J \star \hat{\phi}^{k+\frac{1}{2}}\right], \qquad (5.23) \end{aligned}$$

where $\phi^{-1} \equiv \phi^0$. Of course here the variable $w^{k+\frac{1}{2}}$ is not explicitly needed.

5.4 Unconditional Unique Solvability for Second Order Scheme

We will use the method established in [25] to establish the unconditional solvability of the schemes.

Theorem 5.2. *The second order scheme (5.19) – (5.20) for the nCH equation is discretely mass conservative and uniquely solvable for any time step-size $s > 0$. Likewise, the second order scheme (5.22) – (5.23) for the nAC equation is uniquely solvable for any time step-size $s > 0$.*

Proof. Suppose that ϕ^{k+1}, $w^{k+\frac{1}{2}} \in \mathcal{C}_{m\times n}$ is a periodic solution pair to (5.19) and (5.20). Then summing (5.19) and using the periodic boundary conditions for $w^{k+\frac{1}{2}}$ gives

$$\begin{aligned} h^2\left(\phi^{k+1}-\phi^k\middle\|\mathbf{1}\right) &= sh^2\left(\Delta_h w^{k+\frac{1}{2}}\middle\|\mathbf{1}\right) \\ &= -sh^2\left[D_x w^{k+\frac{1}{2}}\middle\|D_x\mathbf{1}\right]_{\mathrm{ew}} - sh^2\left[D_y w^{k+\frac{1}{2}}\middle\|D_y\mathbf{1}\right]_{\mathrm{ns}} \\ &= 0. \end{aligned} \tag{5.24}$$

Hence $h^2\left(\phi^{k+1}\middle\|\mathbf{1}\right) = h^2\left(\phi^k\middle\|\mathbf{1}\right)$, which clearly is a necessary condition for solvability. Consequently, the set of admissible functions is the hyperplane

$$\mathcal{A}_1 = \left\{\phi\in\mathcal{C}_{m\times n} \;\middle|\; (\phi\|\mathbf{1}) = \left(\phi^k\middle\|\mathbf{1}\right) \text{ and } \phi \text{ is periodic}\right\}.$$

Now, consider the following functional on $\mathcal{A}_1$:

$$G_1^2(\phi) := \frac{1}{2s}\left\|\phi-\phi^k\right\|_H^2 + Q(\phi) + R(\phi), \tag{5.25}$$

where

$$Q(\phi) := \frac{h^2}{4}\left(\frac{\phi^4}{4} + \frac{\phi^3}{3}\phi^k + \frac{\phi^2}{2}\left(\phi^k\right)^2 + \phi\left(\phi^k\right)^3\middle\|\mathbf{1}\right) + \frac{2\left[J\star\mathbf{1}\right]+\gamma_c}{4}\|\phi\|_2^2, \tag{5.26}$$

and

$$
\begin{aligned}
R(\phi) :=& h^2 \left(\phi \middle\| \frac{2\left[J \star \mathbf{1}\right] + \gamma_c}{2} \phi^k \right) \\
& - h^2 \left(\phi \middle\| \left(\left[J_c \star \mathbf{1}\right] + \left[J_e \star \mathbf{1}\right] + \gamma_e\right) \hat{\phi}^{k+\frac{1}{2}} + \left[J \star \hat{\phi}^{k+\frac{1}{2}}\right] \right) .
\end{aligned} \tag{5.27}
$$

Observe that (see, *e.g.*, [25])

$$
w^{k+\frac{1}{2}} = \delta_\phi \left[Q(\phi) + R(\phi)\right], \tag{5.28}
$$

where δ_ϕ is the discrete variational derivative. The functional Q is strictly convex [25]. This, together with the properties of the H inner product and norm given in Sec. 3.2, implies that $G_1^2(\phi)$ is strictly convex and coercive over $\mathcal{A}_1$. Therefore, its unique minimizer $\phi^{k+1} \in \mathcal{A}_1$ satisfies the discrete Euler-Lagrange equation

$$
\delta_\phi G_1^2 \left(\phi^{k+1}\right) = -\Delta_h^{-1} \left(\frac{\phi^{k+1} - \phi^k}{s}\right) + w^{k+\frac{1}{2}} + C = 0, \tag{5.29}
$$

where C is a constant. This is equivalent to

$$
\phi^{k+1} - \phi^k = s \Delta_h w^{k+\frac{1}{2}}, \tag{5.30}
$$

which is just Eq. (5.19). Thus minimizing the strictly convex functional $G_1^2(\phi)$ over the set of admissible functions , the affine space $\mathcal{A}_1$, is the same as solving the second-order convex splitting scheme (5.19) – (5.20). This completes the first part of the proof.

Regarding the solvability of (5.22) – (5.23), consider the functional

$$
G_2^2(\phi) := \frac{1}{2s} \left\|\phi - \phi^k\right\|_2^2 + Q(\phi) + R(\phi). \tag{5.31}
$$

Then $G_2^2(\phi)$ is strictly convex and coercive over the set of admissible functions

$$\mathcal{A}_2 = \{\phi \in \mathcal{C}_{m\times n} \mid \phi \text{ is periodic}\}, \tag{5.32}$$

and its unique minimizer $\phi^{k+1} \in \mathcal{A}_2$ satisfies the discrete Euler-Lagrange equation

$$\delta_\phi G_2^2\left(\phi^{k+1}\right) = \frac{\phi^{k+1} - \phi^k}{s} + w^{k+\frac{1}{2}} = 0, \tag{5.33}$$

which is equivalent to Eq. (5.22). Thus minimizing the strictly convex functional $G_2^2(\phi)$ over the set of admissible functions $\mathcal{A}_2$ is the same as solving the second-order convex splitting scheme (5.22) – (5.23). This completes the second part of the proof. □

5.5 Unconditional Energy and L^4 Stability for the Second Order Scheme

Now we prove the unconditional energy stabilty and $\ell^\infty\left(0, T; \ell^4\right)$ stability for the mass-conserving scheme (5.19) – (5.20) and the non-conserving scheme (5.22) – (5.23). We are going to use the psuedo energy defined as Eq. (4.20).

Theorem 5.3. *Suppose that* $\left\{\phi^{k+1},\, w^{k+\frac{1}{2}}\right\} \in \left[\mathcal{C}_{m\times n}\right]^2$ *is a periodic solution pair to (5.19) – (5.20). Then, for any* $s > 0$*,*

$$\mathcal{F}\left(\phi^k, \phi^{k+1}\right) + s\left\|\nabla_h w^{k+\frac{1}{2}}\right\|_2^2 + R\left(\phi^{k-1}, \phi^k, \phi^{k+1}\right) = \mathcal{F}\left(\phi^{k-1}, \phi^k\right), \tag{5.34}$$

where

$$\begin{aligned} & R\left(\phi^{k-1}, \phi^k, \phi^{k+1}\right) \\ = \; & \frac{[J_c \star \mathbf{1}] + [J_e \star \mathbf{1}] + \gamma_e}{4}\left\|\phi^{k+1} - 2\phi^k + \phi^{k-1}\right\|_2^2 \\ & + \frac{h^2}{4}\left(\left[J \star \left(\phi^{k+1} - 2\phi^k + \phi^{k-1}\right)\right]\middle\|\left[\phi^{k+1} - 2\phi^k + \phi^{k-1}\right]\right). \end{aligned} \tag{5.35}$$

The remainder term, $R\left(\phi^{k-1},\phi^{k},\phi^{k+1}\right)$*, is non-negative, which implies that the psuedo energy is non-increasing,* i.e., $\mathcal{F}\left(\phi^{k},\phi^{k+1}\right) \le \mathcal{F}\left(\phi^{k-1},\phi^{k}\right)$*. Similarly, if* $\left\{\phi^{k+1},\, w^{k+\frac{1}{2}}\right\} \in \left[\mathcal{C}_{m\times n}\right]^2$ *is a periodic solution pair to the scheme (5.22) – (5.23), then, for any* $s>0$*,*

$$\mathcal{F}\left(\phi^{k},\phi^{k+1}\right) + s\left\|w^{k+\frac{1}{2}}\right\|_2^2 + R\left(\phi^{k-1},\phi^{k},\phi^{k+1}\right) = \mathcal{F}\left(\phi^{k-1},\phi^{k}\right), \tag{5.36}$$

which implies that the pseudo energy is non-increasing, i.e.,

$$\mathcal{F}\left(\phi^{k},\phi^{k+1}\right) \le \mathcal{F}\left(\phi^{k-1},\phi^{k}\right). \tag{5.37}$$

Proof. We first note the following identities:

$$h^2\left(\phi^{k+\frac{1}{2}}\chi\left(\phi^{k},\phi^{k+1}\right)\middle\|\phi^{k+1}-\phi^{k}\right) = \frac{1}{4}\left\|\phi^{k+1}\right\|_4^4 - \frac{1}{4}\left\|\phi^{k}\right\|_4^4, \tag{5.38}$$

$$h^2\left(\phi^{k+\frac{1}{2}}\middle\|\phi^{k+1}-\phi^{k}\right) = \frac{1}{2}\left\|\phi^{k+1}\right\|_2^2 - \frac{1}{2}\left\|\phi^{k}\right\|_2^2, \tag{5.39}$$

$$\begin{aligned} -h^2\left(\hat{\phi}^{k+\frac{1}{2}}\middle\|\phi^{k+1}-\phi^{k}\right) \;=\; & -\frac{1}{2}\left\|\phi^{k+1}\right\|_2^2 + \frac{1}{4}\left\|\phi^{k+1}-\phi^{k}\right\|_2^2 \\ & +\frac{1}{2}\left\|\phi^{k}\right\|_2^2 - \frac{1}{4}\left\|\phi^{k}-\phi^{k-1}\right\|_2^2 \\ & +\frac{1}{4}\left\|\phi^{k+1}-2\phi^{k}+\phi^{k-1}\right\|_2^2, \end{aligned} \tag{5.40}$$

and

$$\begin{aligned} & -\left(\left[J\star\hat{\phi}^{k+\frac{1}{2}}\right]\middle\|\phi^{k+1}-\phi^{k}\right) \\ = \; & -\frac{1}{2}\left(\left[J\star\phi^{k+1}\right]\middle\|\phi^{k+1}\right) + \frac{1}{4}\left(\left[J\star\left(\phi^{k+1}-\phi^{k}\right)\right]\middle\|\phi^{k+1}-\phi^{k}\right) \\ & +\frac{1}{2}\left(\left[J\star\phi^{k}\right]\middle\|\phi^{k}\right) - \frac{1}{4}\left(\left[J\star\left(\phi^{k}-\phi^{k-1}\right)\right]\middle\|\phi^{k}-\phi^{k-1}\right) \\ & +\frac{1}{4}\left(\left[J\star\left(\phi^{k+1}-2\phi^{k}+\phi^{k-1}\right)\right]\middle\|\phi^{k+1}-2\phi^{k}+\phi^{k-1}\right). \end{aligned} \tag{5.41}$$

Now, testing Eq. (5.19) with $w^{k+\frac{1}{2}}$, we obtain

$$h^2\left(\phi^{k+1}-\phi^k\middle\|w^{k+\frac{1}{2}}\right)=-s\left\|\nabla_h w^{k+\frac{1}{2}}\right\|_2^2, \tag{5.42}$$

but, considering Eq. (5.20), we have

$$\begin{aligned} h^2\left(\phi^{k+1}-\phi^k\middle\|w^{k+\frac{1}{2}}\right) \;=\;& h^2\left(\phi^{k+\frac{1}{2}}\chi\left(\phi^k,\phi^{k+1}\right)\middle\|\phi^{k+1}-\phi^k\right) \\ &+\left(2\left[J_c\star\mathbf{1}\right]+\gamma_c\right)h^2\left(\phi^{k+\frac{1}{2}}\middle\|\phi^{k+1}-\phi^k\right) \\ &-\left(\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e\right)h^2\left(\hat{\phi}^{k+\frac{1}{2}}\middle\|\phi^{k+1}-\phi^k\right) \\ &-h^2\left(\left[J\star\hat{\phi}^{k+\frac{1}{2}}\right]\middle\|\phi^{k+1}-\phi^k\right)\;. \end{aligned} \tag{5.43}$$

Using identities (5.38) – (5.41) in the last equation, we get

$$\begin{aligned} & h^2\left(\phi^{k+1}-\phi^k\middle\|w^{k+1}\right) \\ =\;& \frac{1}{4}\left\|\phi^{k+1}\right\|_4^4-\frac{1}{4}\left\|\phi^k\right\|_4^4 \\ &+\frac{2\left[J_c\star\mathbf{1}\right]+\gamma_c}{2}\left\|\phi^{k+1}\right\|_2^2-\frac{2\left[J_c\star\mathbf{1}\right]+\gamma_c}{2}\left\|\phi^k\right\|_2^2 \\ &-\frac{\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e}{2}\left\|\phi^{k+1}\right\|_2^2 \\ &+\frac{\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e}{4}\left\|\phi^{k+1}-\phi^k\right\|_2^2 \\ &+\frac{\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e}{2}\left\|\phi^k\right\|_2^2 \\ &-\frac{\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e}{4}\left\|\phi^k-\phi^{k-1}\right\|_2^2 \\ &+\frac{\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]+\gamma_e}{4}\left\|\phi^{k+1}-2\phi^k+\phi^{k-1}\right\|_2^2 \\ &-\frac{h^2}{2}\left(\left[J\star\phi^{k+1}\right]\middle\|\phi^{k+1}\right)+\frac{h^2}{4}\left(\left[J\star\left(\phi^{k+1}-\phi^k\right)\right]\middle\|\phi^{k+1}-\phi^k\right) \\ &+\frac{h^2}{2}\left(\left[J\star\phi^k\right]\middle\|\phi^k\right)-\frac{h^2}{4}\left(\left[J\star\left(\phi^k-\phi^{k-1}\right)\right]\middle\|\phi^k-\phi^{k-1}\right) \\ &+\frac{h^2}{4}\left(\left[J\star\left(\phi^{k+1}-2\phi^k+\phi^{k-1}\right)\right]\middle\|\phi^{k+1}-2\phi^k+\phi^{k-1}\right) \\ =\;& \mathcal{F}\left(\phi^k,\phi^{k+1}\right)-\mathcal{F}\left(\phi^{k-1},\phi^k\right)+R\left(\phi^{k-1},\phi^k,\phi^{k+1}\right). \end{aligned} \tag{5.44}$$

The only remaining piece to show is that $R\left(\phi^{k-1},\phi^{k},\phi^{k+1}\right)\geq 0$. But, by Lem. 3.3.2 and the definition of $R\left(\phi^{k-1},\phi^{k},\phi^{k+1}\right)$, this fact is straightforward. The first result is proven. The proof of the second part is quite similar and is omitted for the sake of brevity. ☐

Corollary 5.5.1. *Suppose that* $\left\{\phi^{k+1},\mu^{k+\frac{1}{2}}\right\}_{k=1}^{\ell}\in\left[\mathcal{C}_{m\times n}\right]^2$ *are a sequence of periodic solutions pairs of the conservative scheme (5.19) – (5.20) or the non-conservative scheme (5.22) – (5.23) with the starting values* ϕ^0 *and* ϕ^{-1}*, where* $\phi^0\equiv\phi^{-1}$*. Then, for any* $1\leq k\leq\ell$*,*

$$\frac{1}{8}\left\|\phi^k\right\|_4^4 \leq F\left(\phi^0\right)+\frac{\left(\gamma_c-\gamma_e-2\left[J_e\star\mathbf{1}\right]\right)^2}{2}|\Omega|, \tag{5.45}$$

$$\frac{1}{2}\left\|\phi^k\right\|_2^2 \leq F\left(\phi^0\right)+\frac{\left(\gamma_c-\gamma_e-2\left[J_e\star\mathbf{1}\right]-1\right)^2}{2}|\Omega|. \tag{5.46}$$

Proof. By virtue of the last theorem, and since $\phi^{-1}\equiv\phi^0$, we have the chain of inequalities

$$F\left(\phi^k\right)\leq\mathcal{F}\left(\phi^k\right)\leq\mathcal{F}\left(\phi^{k-1}\right)\leq\cdots\leq\mathcal{F}\left(\phi^0\right)=F\left(\phi^0\right). \tag{5.47}$$

By Lem. 4.3.1, the result is proved. ☐

Theorem 5.4. *Let* $\Phi(x,y)$ *be a sufficiently regular, periodic function on* $\Omega=(0,L_{x_1})\times(0\times L_{x_2})$ *and* $\phi_{i,j}^0:=\Phi(p_i,p_j)$*. Suppose* E *is the continuous energy (1.13) and* F *is the discrete energy (4.19). Let* $\phi_{i,j}^k\in\mathcal{C}_{m\times n}$ *be the* k^{th} *periodic solution,* $1\leq k\leq\ell$*, of the conservative scheme (5.19) – (5.20) or the non-conservative scheme (5.22) – (5.23) with the starting values* $\phi^0\equiv\phi^{-1}$*. There exist constants,* $C_1,\dots C_4>0$*, which are independent of* h *and* s*, such that*

$$\max_{1\leq k\leq\ell}\left\|\phi^k\right\|_4 \leq C_1. \tag{5.48}$$

$$\max_{1\leq k\leq\ell}\left\|\phi^k\right\|_2 \leq C_2. \tag{5.49}$$

In the case of (5.19) – (5.20), we have

$$\sqrt{s\sum_{k=1}^{\ell}\left\|\nabla_h w^{k+\frac{1}{2}}\right\|_2^2} \le C_3, \tag{5.50}$$

and, in the case of (5.22) – (5.23), we have

$$\sqrt{s\sum_{k=1}^{\ell}\left\|w^{k+\frac{1}{2}}\right\|_2^2} \le C_4. \tag{5.51}$$

Proof. Since the discrete energy F is consistent with E,

$$F\left(\phi^0\right) \le E\left(\Phi\right) + Ch^2 \le E\left(\Phi\right) + C|\Omega|, \tag{5.52}$$

where $C > 0$ is independent of h. Invoking Cor. 5.5.1 and using a second consistency argument on the discrete convolution $[J_e \star \mathbf{1}]$, for all $1 \le k \le \ell$, we have

$$\begin{aligned} \frac{1}{8}\left\|\phi^k\right\|_4^4 &\le F\left(\phi^0\right) + \frac{\left(\gamma_c - \gamma_e - 2\left[J_e \star \mathbf{1}\right]\right)^2}{2}|\Omega|, \\ &\le E\left(\Phi\right) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right)\right)^2}{2}|\Omega| + C|\Omega|, \end{aligned} \tag{5.53}$$

and

$$\begin{aligned} \frac{1}{2}\left\|\phi^k\right\|_2^2 &\le F\left(\phi^0\right) + \frac{\left(\gamma_c - \gamma_e - 2\left[J_e \star \mathbf{1}\right] - 1\right)^2}{2}|\Omega| \\ &\le E\left(\Phi\right) + \frac{\left(\gamma_c - \gamma_e - 2\left(J_e * 1\right) - 1\right)^2}{2}|\Omega| + C|\Omega|. \end{aligned} \tag{5.54}$$

The right-hand-sides are clearly independent of h and s, and the first two *a priori* bounds are proven. The third and fourth follow by summing the estimates in Thm. 5.3, to yeild

$$s\sum_{k=1}^{\ell}\left\|\nabla_h w^{k+\frac{1}{2}}\right\|_2^2 \le F\left(\phi^0\right) \tag{5.55}$$

in the case of the nCH scheme, and

$$s\sum_{k=1}^{\ell}\left\|w^{k+\frac{1}{2}}\right\|_2^2 \leq F\left(\phi^0\right) \tag{5.56}$$

in the case of the nAC scheme, and using the consistency arguments as above. □

5.6 Local-in-Time Convergence and L^∞ bound for nAC Equation

In this section we prove the local-in-time ℓ^2 convergence of scheme for the nAC equation, (5.22) – (5.23). We need a couple of technical lemmas before we begin.

Lemma 5.6.1. *Let ℓ be a positive integer. If $\phi^k \in \mathcal{C}_{m\times n}$, $0 \leq k \leq \ell$, with $\phi^0 \equiv \phi^1$, then*

$$\sum_{k=1}^{\ell}\left(\phi^{k+\frac{1}{2}}\middle\|\hat{\phi}^{k+\frac{1}{2}}\right) \leq 2\sum_{k=1}^{\ell}\left(\phi^k\middle\|\phi^k\right) + \frac{1}{2}\left(\phi^{\ell+1}\middle\|\phi^{\ell+1}\right), \tag{5.57}$$

and

$$\sum_{k=1}^{\ell}\left(\phi^{k+\frac{1}{2}}\middle\|\phi^{k+\frac{1}{2}}\right) \leq \sum_{k=1}^{\ell}\left(\phi^k\middle\|\phi^k\right) + \frac{1}{2}\left(\phi^{\ell+1}\middle\|\phi^{\ell+1}\right). \tag{5.58}$$

Proof. First we prove Eq. (5.57). From the definitions for $\phi^{k+\frac{1}{2}}$, $\hat{\phi}^{k+\frac{1}{2}}$ and the identity $\pm ab \leq \frac{1}{2}a^2 + \frac{1}{2}b^2$,

$$\begin{aligned}
\left(\phi^{k+\frac{1}{2}}\middle\|\hat{\phi}^{k+\frac{1}{2}}\right) = &\left(\frac{1}{2}\phi^{k+1} + \frac{1}{2}\phi^k\middle\|\frac{3}{2}\phi^k - \frac{1}{2}\phi^{k-1}\right)\\
=&\frac{3}{4}\left(\phi^{k+1}\middle\|\phi^k\right) + \frac{3}{4}\left(\phi^k\middle\|\phi^k\right) - \frac{1}{4}\left(\phi^{k+1}\middle\|\phi^{k-1}\right) - \frac{1}{4}\left(\phi^k\middle\|\phi^{k-1}\right)\\
\leq&\frac{3}{8}\left(\phi^{k+1}\middle\|\phi^{k+1}\right) + \frac{3}{8}\left(\phi^k\middle\|\phi^k\right) + \frac{3}{4}\left(\phi^k\middle\|\phi^k\right) + \frac{1}{8}\left(\phi^{k+1}\middle\|\phi^{k+1}\right)\\
&+ \frac{1}{8}\left(\phi^{k-1}\middle\|\phi^{k-1}\right) + \frac{1}{8}\left(\phi^k\middle\|\phi^k\right) + \frac{1}{8}\left(\phi^{k-1}\middle\|\phi^{k-1}\right)\\
=&\frac{1}{2}\left(\phi^{k+1}\middle\|\phi^{k+1}\right) + \frac{5}{4}\left(\phi^k\middle\|\phi^k\right) + \frac{1}{4}\left(\phi^{k-1}\middle\|\phi^{k-1}\right).
\end{aligned} \tag{5.59}$$

Summing and using $\phi^0 \equiv \phi^1$,

$$\begin{aligned}
\sum_{k=1}^{\ell} \left(\phi^{k+\frac{1}{2}} \middle\| \hat{\phi}^{k+\frac{1}{2}}\right) \leq & \frac{1}{2}\sum_{k=1}^{\ell} \left(\phi^{k+1} \| \phi^{k+1}\right) + \frac{5}{4}\sum_{k=1}^{\ell} \left(\phi^{k} \| \phi^{k}\right) + \frac{1}{4}\sum_{k=1}^{\ell} \left(\phi^{k-1} \| \phi^{k-1}\right) \\
= & \frac{1}{2}\sum_{k=2}^{\ell+1} \left(\phi^{k} \| \phi^{k}\right) + \frac{5}{4}\sum_{k=1}^{\ell} \left(\phi^{k} \| \phi^{k}\right) + \frac{1}{4}\sum_{k=0}^{\ell-1} \left(\phi^{k} \| \phi^{k}\right) \\
= & 2\sum_{k=1}^{\ell} \left(\phi^{k} \| \phi^{k}\right) + \frac{1}{2}\left(\phi^{\ell+1} \| \phi^{\ell+1}\right) - \frac{1}{4}\left(\phi^{\ell} \| \phi^{\ell}\right) - \frac{1}{4}\left(\phi^{1} \| \phi^{1}\right) \\
\leq & 2\sum_{k=0}^{\ell} \left(\phi^{k} \| \phi^{k}\right) + \frac{1}{2}\left(\phi^{\ell+1} \| \phi^{\ell+1}\right) \ .
\end{aligned} \tag{5.60}$$

The proof of Eq. (5.58) is even simpler and is omitted. □

Lemma 5.6.2. *Let ℓ be a positive integer and assume J is defined as in Eq. (4.19). If $\phi^k \in \mathcal{C}_{m\times n}$, $0 \le k \le \ell$, is periodic, with $\phi^0 \equiv \phi^1$, then*

$$\begin{aligned}
\sum_{k=1}^{\ell} \left(\left[J \star \hat{\phi}^{k+\frac{1}{2}}\right] \middle\| \phi^{k+\frac{1}{2}}\right) \leq & 2\left([J_c \star 1] + [J_e \star 1]\right) \sum_{k=1}^{\ell} \left(\phi^{k} \| \phi^{k}\right) \\
& + \frac{[J_c \star 1] + [J_e \star 1]}{2}\left(\phi^{\ell+1} \| \phi^{\ell+1}\right) .
\end{aligned} \tag{5.61}$$

Proof. Using the definitions of $\phi^{k+\frac{1}{2}}$ and $\hat{\phi}^{k+\frac{1}{2}}$,

$$\begin{aligned}
\left(\left[J \star \hat{\phi}^{k+\frac{1}{2}}\right] \middle\| \phi^{k+\frac{1}{2}}\right) = & \left(\left[J \star \left(\frac{3}{2}\phi^{k} - \frac{1}{2}\phi^{k-1}\right)\right] \middle\| \frac{1}{2}\phi^{k+1} + \frac{1}{2}\phi^{k}\right) \\
= & \frac{3}{4}\left(\left[J \star \phi^{k}\right] \| \phi^{k+1}\right) + \frac{3}{4}\left(\left[J \star \phi^{k}\right] \| \phi^{k}\right) \\
& - \frac{1}{4}\left(\left[J \star \phi^{k-1}\right] \| \phi^{k+1}\right) - \frac{1}{4}\left(\left[J \star \phi^{k-1}\right] \| \phi^{k}\right) .
\end{aligned} \tag{5.62}$$

Using $J = J_c - J_e$, the linearity of the discrete convolution $[\,\cdot \star \cdot\,]$, and Prop. 3.3.2,

$$\begin{aligned}
&\left(\left[J \star \hat{\phi}^{k+\frac{1}{2}}\right] \middle\| \phi^{k+\frac{1}{2}}\right) \\
\leq &\frac{3\left([J_c \star 1] + [J_e \star 1]\right)}{8}\left(\phi^{k+1}\middle\|\phi^{k+1}\right) + \frac{3\left([J_c \star 1] + [J_e \star 1]\right)}{8}\left(\phi^{k}\middle\|\phi^{k}\right) \\
&+ \frac{3\left([J_c \star 1] + [J_e \star 1]\right)}{4}\left(\phi^{k}\middle\|\phi^{k}\right) + \frac{\left([J_c \star 1] + [J_e \star 1]\right)}{8}\left(\phi^{k+1}\middle\|\phi^{k+1}\right) \\
&+ \frac{\left([J_c \star 1] + [J_e \star 1]\right)}{8}\left(\phi^{k-1}\middle\|\phi^{k-1}\right) + \frac{\left([J_c \star 1] + [J_e \star 1]\right)}{8}\left(\phi^{k}\middle\|\phi^{k}\right) \\
&+ \frac{\left([J_c \star 1] + [J_e \star 1]\right)}{8}\left(\phi^{k-1}\middle\|\phi^{k-1}\right). \qquad (5.63)
\end{aligned}$$

Proceeding as in the proof of Lem. 5.6.1, we have

$$\begin{aligned}
\sum_{k=1}^{\ell}\left(\left[J \star \hat{\phi}^{k+\frac{1}{2}}\right] \middle\| \phi^{k+\frac{1}{2}}\right) \leq &2\left([J_c \star 1] + [J_e \star 1]\right)\sum_{k=1}^{\ell}\left(\phi^{k}\middle\|\phi^{k}\right) \\
&+ \frac{[J_c \star 1] + [J_e \star 1]}{2}\left(\phi^{\ell+1}\middle\|\phi^{\ell+1}\right). \qquad (5.64)
\end{aligned}$$

□

Theorem 5.5. *Given smooth, periodic initial data $\Phi(x, y, t = 0)$, suppose the unique, smooth, periodic solution for nAC equation (1.3) is given by $\Phi(x, y, t)$ on Ω for $0 < t \leq T$, for some $T < \infty$. Define $\Phi^k_{i,j} := \Phi(p_i, p_j, ks)$, and $e^k_{i,j} := \Phi^k_{i,j} - \phi^k_{i,j}$, where $\phi^k_{i,j} \in \mathcal{C}_{m\times n}$ is k^{th} periodic solution of (5.22) – (5.23) with $\phi^0_{i,j} := \Phi^0_{i,j}$ and $\phi^1_{i,j} := \Phi^1_{i,j}$. Then, provided s is sufficiently small, $s \leq h$, for some $M > 0$,*

$$\left\|e^{\ell}\right\|_2 \leq C\left(h^2 + s^2\right), \qquad (5.65)$$

where $\ell \cdot s = T$, for some $C > 0$ that is independent of h and s. Furthermore, $\left\|\phi^k\right\|_\infty < \infty$.

Proof. The continuous function Φ solves the discrete equations

$$\Phi^{k+1} - \Phi^{k} = -s w^{k+\frac{1}{2}}\left(\Phi^{k+1}, \Phi^{k}\right) + s\tau^{k+1} \tag{5.66}$$

$$\begin{aligned} w^{k+\frac{1}{2}}\left(\Phi^{k}, \Phi^{k+1}\right) &= \Phi^{k+\frac{1}{2}}\chi(\Phi^{k}, \Phi^{k+1}) + \left[2\left[J_c \star \mathbf{1}\right] + \gamma_c\right]\Phi^{k+\frac{1}{2}} \\ &\quad - \left[\left[J_c \star \mathbf{1}\right] + \left[J_e \star \mathbf{1}\right] + \gamma_e\right]\hat{\Phi}^{k+\frac{1}{2}} - \left[J \star \hat{\Phi}^{k+\frac{1}{2}}\right], \end{aligned} \tag{5.67}$$

where τ^{k+1} is the local truncation error, which satisfies

$$\left|\tau_{i,j}^{k+1}\right| \leq M_2\left(h^2 + s^2\right), \tag{5.68}$$

for all i, j, and k for some $M_2 \geq 0$ that depends only on Φ, T, L_{x_1}, and L_{x_2}. As in [Bao and Cai], choose a cutoff function $\alpha \in C^{\infty}[0,\infty)$ such that $0 \leq \alpha(\rho) \leq 1$ for all $\rho \in [0,\infty)$ and

$$\alpha(\rho) = \begin{cases} 1 & 0 \leq \rho \leq 1 \\ \varXi[0,1] & 1 \leq \rho \leq 2 \\ 0 & 2 \leq \rho \end{cases}. \tag{5.69}$$

Define

$$F_{M_1}(\rho) = \alpha\left(\frac{\rho}{M_1}\right)\rho \tag{5.70}$$

and

$$\widetilde{\chi}(\phi, \psi) := \frac{1}{2}\left(F_{M_1}\left(\phi^2\right) + F_{M_1}\left(\psi^2\right)\right). \tag{5.71}$$

One can now create a new nonlocal Allen-Cahn equation: Find Ψ such that

$$\partial_t \Psi = -\widetilde{w}(\Psi), \tag{5.72}$$

$$\widetilde{w}(\Psi) := \widetilde{\chi}(\Psi, \Psi)\Psi + (\gamma_c - \gamma_e)\Psi + (J * 1)\Psi - J * \Psi. \tag{5.73}$$

Assuming that $M_1 = 2\left(1 + \|\Phi\|_{L^{\infty}(0,T;L^{\infty})}\right)^2 < \infty$ and $\Psi(\,\cdot\,,0) = \Phi(\,\cdot\,,0)$, then $\Psi \equiv \Phi$. To this new Allen-Cahn equation we can also derive the corresponding convex splitting scheme:

$$\psi^{k+1} - \psi^{k} = - s\widetilde{w}^{k+\frac{1}{2}}\left(\psi^{k}, \psi^{k+1}\right), \tag{5.74}$$

$$\begin{aligned}\widetilde{w}^{k+\frac{1}{2}}\left(\psi^{k}, \psi^{k+1}\right) :=& \widetilde{\chi}\left(\psi^{k}, \psi^{k+1}\right)\psi^{k+\frac{1}{2}} + \left(2\left[J_c \star \mathbf{1}\right] + \gamma_c\right)\psi^{k+\frac{1}{2}} \\ &- \left(\left[J_c \star \mathbf{1}\right] + \left[J_e \star \mathbf{1}\right] + \gamma_e\right)\hat{\psi}^{k+\frac{1}{2}} - \left[J \star \hat{\psi}^{k+\frac{1}{2}}\right].\end{aligned} \tag{5.75}$$

Thus,

$$\Psi^{k+1} - \Psi^{k} = -s\widetilde{w}^{k+\frac{1}{2}}\left(\Psi^{k}, \Psi^{k+1}\right) + s\tau^{k+1}. \tag{5.76}$$

Subtracting Eq. (5.74) from Eq. (5.76),

$$\varepsilon^{k+1} - \varepsilon^{k} = -s\left[\widetilde{w}^{k+\frac{1}{2}}\left(\Psi^{k}, \Psi^{k+1}\right) - \widetilde{w}^{k+\frac{1}{2}}\left(\psi^{k}, \psi^{k+1}\right)\right] + s\tau^{k+1}, \tag{5.77}$$

where ε^{k} is defined as

$$\varepsilon^{k} := \Psi^{k} - \psi^{k}. \tag{5.78}$$

Multiplying both sides by of Eq. (5.77) $h^2\varepsilon^{k+\frac{1}{2}}$ and summing over i and j, we have

$$\begin{aligned}\left\|\varepsilon^{k+1}\right\|_2^2 - \left\|\varepsilon^{k}\right\|_2^2 =& - sh^2\left(\widetilde{\chi}\left(\Psi^{k}, \Psi^{k+1}\right)\Psi^{k+\frac{1}{2}} - \widetilde{\chi}\left(\psi^{k}, \psi^{k+1}\right)\psi^{k+\frac{1}{2}}\middle\|\varepsilon^{k+\frac{1}{2}}\right) \\ &- sh^2\left(2\left[J_c \star \mathbf{1}\right] + \gamma_c\right)\left(\varepsilon^{k+\frac{1}{2}}\middle\|\varepsilon^{k+\frac{1}{2}}\right) \\ &+ sh^2\left(\left[J_c \star \mathbf{1}\right] + \left[J_e \star \mathbf{1}\right] + \gamma_e\right)\left(\hat{\varepsilon}^{k+\frac{1}{2}}\middle\|\varepsilon^{k+\frac{1}{2}}\right) \\ &+ sh^2\left(\left[J \star \hat{\varepsilon}^{k+\frac{1}{2}}\right]\middle\|\varepsilon^{k+\frac{1}{2}}\right) \\ &+ sh^2\left(\tau^{k+1}\middle\|\varepsilon^{k+\frac{1}{2}}\right),\end{aligned}$$

where $\hat{\varepsilon}^{k+\frac{1}{2}} = \frac{3}{2}\varepsilon^k - \frac{1}{2}\varepsilon^{k-1}$, as usual. By construction of the cutoff function,

$$\begin{aligned}
&- \left(\widetilde{\chi}\left(\Psi^k, \Psi^{k+1}\right) \Psi^{k+\frac{1}{2}} - \widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \psi^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\
=& - \left(\widetilde{\chi}\left(\Psi^k, \Psi^{k+1}\right) \Psi^{k+\frac{1}{2}} - \widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \psi^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\
&+ \left(-\widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \Psi^{k+\frac{1}{2}} + \widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \Psi^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\
=& - \left(\widetilde{\chi}\left(\Psi^k, \Psi^{k+1}\right) \Psi^{k+\frac{1}{2}} - \widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \Psi^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\
&- \left(\widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \Psi^{k+\frac{1}{2}} - \widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \psi^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \ .
\end{aligned} \tag{5.79}$$

By the definition of cutoff function

$$\left|\widetilde{\chi}\left(\psi^k, \psi^{k+1}\right)\right| \leq M_1 \ , \tag{5.80}$$

$$\left|\widetilde{\chi}\left(\Psi^k, \Psi^{k+1}\right) - \widetilde{\chi}\left(\psi^k, \psi^{k+1}\right)\right| \leq C_{M_1} \left|\varepsilon^{k+\frac{1}{2}}\right| \ , \tag{5.81}$$

where $C_{M_1} < \infty$ is a constant depend on M_1. Thus by denoting $M_4 := \left(C_{M_1} \|\Phi\|_{L^\infty(0,T;L^\infty)} + M_1\right)$,

$$\begin{aligned}
&- \left(\widetilde{\chi}\left(\Psi^k, \Psi^{k+1}\right) \Psi^{k+\frac{1}{2}} - \widetilde{\chi}\left(\psi^k, \psi^{k+1}\right) \psi^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\
\leq& C_{M_1} \|\Phi\|_{L^\infty(0,T;L^\infty)} \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) + M_1 \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\
=& M_4 \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \ .
\end{aligned} \tag{5.82}$$

Also notice that

$$sh^2 \left(\tau^{k+1} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \leq s\frac{M_2}{2} \left(h^2 + s^2\right)^2 + \frac{1}{2}h^2 s \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \ . \tag{5.83}$$

By combining the above results

$$\begin{aligned}\left\|\varepsilon^{k+1}\right\|_2^2 - \left\|\varepsilon^k\right\|_2^2 \leq & sh^2 M_4 \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) + sh^2 \left([J_c \star \mathbf{1}] + [J_e \star \mathbf{1}] + \gamma_e\right) \left(\hat{\varepsilon}^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\ & + sh^2 \left(\left[J \star \hat{\varepsilon}^{k+\frac{1}{2}}\right] \middle\| \varepsilon^{k+\frac{1}{2}}\right) + \frac{sM_2}{2}\left(h^2 + s^2\right)^2 \\ & + \frac{1}{2} sh^2 \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right).\end{aligned}$$

Summing over k and using $\varepsilon^0 \equiv \varepsilon^1 \equiv 0$, we have

$$\begin{aligned}\left\|\varepsilon^{\ell+1}\right\|_2^2 \leq & sh^2 M_4 \sum_{k=1}^{\ell} \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\ & + sh^2 \sum_{k=1}^{\ell} \left([J_c \star 1] + [J_e \star 1] + \gamma_e\right) \left(\hat{\varepsilon}^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\ & + h^2 s \sum_{k=1}^{\ell} \left(\left[J \star \hat{\varepsilon}^{k+\frac{1}{2}}\right] \middle\| \varepsilon^{k+\frac{1}{2}}\right) \\ & + \frac{sM_2}{2} \sum_{k=1}^{\ell} \left(h^2 + s^2\right)^2 + \frac{sh^2}{2} \sum_{k=1}^{\ell} \left(\varepsilon^{k+\frac{1}{2}} \middle\| \varepsilon^{k+\frac{1}{2}}\right).\end{aligned}$$

Therefore, by Lems. 5.6.1 and 5.6.2,

$$\begin{aligned}
\left\|\varepsilon^{\ell+1}\right\|_2^2 \leq & s\left(M_4+\frac{1}{2}\right)\sum_{k=1}^{\ell}\left\|\varepsilon^k\right\|_2^2+\frac{s}{2}\left(M_4+\frac{1}{2}\right)\left\|\varepsilon^{\ell+1}\right\|_2^2 \\
& + s\left(4\left[J_c\star\mathbf{1}\right]+4\left[J_e\star\mathbf{1}\right]+2\gamma_e\right)\sum_{k=1}^{\ell}\left\|\varepsilon^k\right\|_2^2 \\
& + s\left(\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]\right)\left\|\varepsilon^{\ell+1}\right\|_2^2+\frac{sM_2}{2}\sum_{k=1}^{\ell}\left(h^2+s^2\right)^2 \\
= & s\left(M_4+\frac{1}{2}+4\left[J_c\star\mathbf{1}\right]+4\left[J_e\star\mathbf{1}\right]+2\gamma_e\right)\sum_{k=1}^{\ell}\left\|\varepsilon^k\right\|_2^2 \\
& + s\left(\frac{M_4}{2}+\frac{1}{4}+\left[J_c\star\mathbf{1}\right]+\left[J_e\star\mathbf{1}\right]\right)\left\|\varepsilon^{\ell+1}\right\|_2^2+\frac{sM_2}{2}\sum_{k=1}^{\ell}\left(h^2+s^2\right)^2 \\
\leq & s\left(M_4+\frac{1}{2}+4\left[J_c\star\mathbf{1}\right]+4\left[J_e\star\mathbf{1}\right]+2\gamma_e\right)\sum_{k=1}^{\ell}\left\|\varepsilon^k\right\|_2^2 \\
& + s\left(M_4+\frac{1}{2}+4\left[J_c\star\mathbf{1}\right]+4\left[J_e\star\mathbf{1}\right]+2\gamma_e\right)\left\|\varepsilon^{\ell+1}\right\|_2^2 \\
& + \frac{sM_2}{2}\sum_{k=1}^{\ell}\left(h^2+s^2\right)^2 . \qquad (5.84)
\end{aligned}$$

Set $M_3 := M_4+\frac{1}{2}+4\left[J_c\star\mathbf{1}\right]+4\left[J_e\star\mathbf{1}\right]+2\gamma_e$, and suppose that $s<\min\left\{M_3^{-1},1\right\}$. We arrive at

$$\left\|\varepsilon^{\ell+1}\right\|_2^2 \leq \frac{sM_3}{1-sM_3}\sum_{k=1}^{\ell}\left\|\varepsilon^k\right\|_2^2+\frac{M_2}{2}\sum_{k=1}^{\ell}\left(h^2+s^2\right)^2 \ . \qquad (5.85)$$

An application of a discrete Gronwall inequality yields

$$\left\|\varepsilon^{\ell+1}\right\|_2^2 \leq \frac{M_2}{2(1-sM_3)}\left(1+\frac{sM_3}{1-sM_3}\right)^{\ell}\left(h^2+s^2\right)^2 . \qquad (5.86)$$

Thus

$$\left\|\varepsilon^{\ell+1}\right\|_2 \leq C\left(h^2+s^2\right). \qquad (5.87)$$

Using the inverse inequality,

$$\left\|\varepsilon^{\ell+1}\right\|_\infty \leq \frac{1}{h}\left\|\varepsilon^{\ell+1}\right\|_2, \tag{5.88}$$

if $s \leq h$, we find

$$\left\|\varepsilon^{\ell+1}\right\|_\infty \leq 2Ch\ . \tag{5.89}$$

This implies

$$\left\|\psi^{\ell+1}\right\|_\infty \leq \left\|\Psi^{\ell+1}\right\|_\infty + \left\|\varepsilon^{\ell+1}\right\|_\infty \leq \left\|\Psi^{\ell+1}\right\|_\infty + 2Ch. \tag{5.90}$$

Therefore, there exists $h_0 > 0$, such that for any $h \leq h_0$,

$$\left\|\psi^{\ell+1}\right\|_\infty \leq (M_1)^{\frac{1}{2}}\ . \tag{5.91}$$

Thus $\psi = \phi$ and $\varepsilon = e$. □

Chapter 6

Numerical Simulations

6.1 Overview

In this chapter we present numerical simulations for schemes we proposed in Chap. 4 and 5. Our contribution in this part includes the numerical verification of the reliability of schemes and the numerical simulation of nucleation phenomena.

This chapter will be organized in following way: in Sec. 6.2 we discuss the details of highly efficient multigrid solver; in Sec. 6.3 we present the numerical test verifying the convergence of schemes and their order; in Sec. 6.4 we present the numerical test verifying the energy dissipation of schemes; in Sec. 6.5 we discuss nucleation phenomena.

6.2 Multigrid Solver

In this section we discuss the details of the highly efficient stable multi-grid solver. The main structure of the solver is borrowed from results in [40], we modified it to simulate nCH and nAC equations. Herein we only present the first order solver for nCH equation, the rest solvers have same structure, thus we skip them in this dissertation.

In detail, the scheme (4.38) is the following: find ϕ^{k+1} and $\tilde{w}^{k+1}$ in $\mathcal{C}_{m\times n}$ with periodic boundary conditions whose components solve

$$
\begin{aligned}
\phi_{i,j}^{k+1} - s\, d_x \left(D_x \tilde{w}^{k+1}\right)_{i,j} - s\, d_y \left(D_y \tilde{w}^{k+1}\right)_{i,j} &= \phi_{i,j}^{k} \,, && (6.1)\\
\tilde{w}_{i,j}^{k+1} - \left(\phi_{i,j}^{k+1}\right)^3 - (2\,[J_c \star 1] + \gamma_c)\phi_{i,j}^{k+1} &= -([J_c \star 1] + [J_e \star 1] + \gamma_e)\phi_{i,j}^{k} \\
&\quad - \left[J \star \phi^k\right]_{i,j} \,. && (6.2)
\end{aligned}
$$

We use a nonlinear FAS multigrid method to solve the system (6.1) – (6.2) efficiently. This involves defining operator and source terms, which we do as follows. Let $\boldsymbol{\phi} = (\phi, \tilde{w})^T$. Define the $2 \times m \times n$ nonlinear operator $\mathbf{N} = (N^{(1)}, N^{(2)})^T$ as

$$
\begin{aligned}
N_{i,j}^{(1)}(\boldsymbol{\phi}) &= \phi_{i,j} - s\, d_x \left(D_x \tilde{w}\right)_{i,j} - s\, d_y \left(D_y \tilde{w}\right)_{i,j} \,, && (6.3)\\
N_{i,j}^{(2)}(\boldsymbol{\phi}) &= \tilde{w}_{i,j} - \left(\phi_{i,j}^{k+1}\right)^3 - (2\,[J_c \star 1] + \gamma_c)\phi_{i,j}^{k+1} \,, && (6.4)
\end{aligned}
$$

and the $2 \times m \times n$ source $\mathbf{S} = (S^{(1)}, S^{(2)})^T$ as

$$
S_{i,j}^{(1)}(\boldsymbol{\phi}) = \phi_{i,j} \,, \qquad S_{i,j}^{(2)}(\boldsymbol{\phi}) = -([J_c \star 1] + [J_e \star 1] + \gamma_e)\phi_{i,j} - [J \star \phi]_{i,j} \,. \qquad (6.5)
$$

Then, of course, Eqs. (6.1) – (6.2) are equivalent to $\mathbf{N}(\boldsymbol{\phi}^{k+1}) = \mathbf{S}(\boldsymbol{\phi}^k)$. Notice that the operator $\mathbf{N}$ depends upon the time step k, because its definition involves the solution ϕ^k. To keep the discussion below as concise as possible, we will neglect this minor detail.

Remark 6.2.1. *It should be emphasized that the convex splitting formation in the scheme (4.38) is crucial in this solver. The current splitting allow us to put the entire numerical convolution calculation into the source term, thus we only need to calculate it once for every time step instead of repeating the expensive calculation in the iteration. It also allow the scheme to adopt the well developed results of FAS multigrid scheme. If the numerical convolution is in the operator, it may even unfeasible to form the smoothing scheme.*

We will describe a somewhat standard nonlinear FAS multigrid scheme for solving the vector equation $\mathbf{N}(\boldsymbol{\phi}^{k+1}) = \mathbf{S}(\boldsymbol{\phi}^k)$. Here we will sketch only the important points of the algorithm; the reader is referred to Trottenberg *et al.* [36, Sec. 5.3] for complete details. To begin we need to discuss a smoothing operator for generating *smoothed* approximate solutions of $\mathbf{N}(\boldsymbol{\phi}) = \mathbf{S}$. The action of this operator is represented as

$$\bar{\boldsymbol{\phi}} = \text{Smooth}\left(\lambda, \boldsymbol{\phi}, \mathbf{N}, \mathbf{S}\right), \tag{6.6}$$

where $\boldsymbol{\phi}$ is an approximate solution prior to smoothing, $\bar{\boldsymbol{\phi}}$ is the smoothed approximation, and λ is the number of smoothing sweeps. For smoothing we use a nonlinear Gauß-Seidel method with Red-Black ordering. In what follows, to simplify the discussion, we give the details of the relaxation using the simpler lexicographic ordering. Let ℓ be the index for the lexicographic Gauß-Seidel. (Note that the smoothing index ℓ in the following should not be confused with the time step index k.) The Gauß-Seidel smoothing is as follows: for every (i,j), stepping lexicographically from $(1,1)$ to (m,n), find $\phi_{i,j}^{\ell+1}$ and $\tilde{w}_{i,j}^{\ell+1}$ that solve

$$\phi_{i,j}^{\ell+1} + \frac{4s}{h^2}\tilde{w}_{i,j}^{\ell+1} = S_{i,j}^{(1)}\left(\boldsymbol{\phi}^k\right) + \frac{s}{h^2}\Big(\tilde{w}_{i+1,j}^{\ell} + \tilde{w}_{i-1,j}^{\ell+1} + \tilde{w}_{i,j+1}^{\ell} + \tilde{w}_{i,j-1}^{\ell+1}\Big)\,, \tag{6.7}$$

$$\Big(-3\left(\phi_{i,j}^{\ell}\right)^2 - \left(2\left[J_c \star 1\right] + \gamma_c\right)\Big)\phi_{i,j}^{\ell+1} + \tilde{w}_{i,j}^{\ell+1} = S_{i,j}^{(2)}\left(\boldsymbol{\phi}^k\right) - 2\left(\phi_{i,j}^{\ell}\right)^3\,. \tag{6.8}$$

Note that we have linearized the cubic term using a local Newton approximation, but otherwise this is a standard vector application of block Gauß-Seidel. The 2×2 linear system defined by (6.7) – (6.8) is unconditionally solvable (the determinant of the coefficient matrix is always positive in this case). We use Cramer's Rule to obtain $\phi_{i,j}^{\ell+1}$ and $\tilde{w}_{i,j}^{\ell+1}$.

One full block Gauß-Seidel sweep has concluded when we have stepped lexicographically through all the grid points, from $(1,1)$ to (m,n). When λ full smoothing sweeps has completed the vector result is labeled $\bar{\boldsymbol{\phi}}$, as in Eq. (6.6), and the action of the smoothing operator is complete.

Multigrid works on a hierarchy of grids. We denote the grid level by the index n, where $n_{\min} \le n \le n_{\max}$, $n_{\max}$ is the index for the finest grid, and $n_{\min}$ is the index for the coarsest grid. We need operators for communicating information from coarse levels to fine levels, and *vice versa*. By $\mathbf{I}_n^{n-1}$ we denote the restriction operator, which transfers fine grid functions, with grid index n, to the coarse grid, indexed by $n-1$. By $\mathbf{I}_{n-1}^{n}$ we denote the prolongation operator, which transfers coarse grid functions (level $n-1$) to the fine grid (level n). Here we work on cell-centered grids. The restriction operator is defined by cell-center averaging; for the prolongation operator we use piece-wise constant interpolation [36, Sec. 2.8.4].

Now we are in a position to define the recursive FAS V-Cycle operator, which is the heart of our muligrid solver. In the following the subscript n is used to denote grid-level n operators, data, *et cetera*, and the superscript m is the V-Cycle loop index.

RECURSIVE FAS V-CYCLE OPERATOR

$$\boldsymbol{\phi}_n^{k+1,m+1} = \text{FASVcycle}\left(n, \boldsymbol{\phi}_n^{k+1,m}, \mathbf{N}_n, \mathbf{S}_n, \lambda\right) \tag{6.9}$$

1. Pre-smoothing:
   - Compute a smoothed approximation $\bar{\boldsymbol{\phi}}_n$:

$$\bar{\boldsymbol{\phi}}_n = \text{Smooth}\left(\lambda, \boldsymbol{\phi}_n^{k+1,m}, \mathbf{N}_n, \mathbf{S}_n\right). \tag{6.10}$$

2. Coarse-grid correction:
   - Compute coarse-level initial iterate:

$$\bar{\boldsymbol{\phi}}_{n-1} = \mathbf{I}_n^{n-1}\bar{\boldsymbol{\phi}}_n \tag{6.11}$$

   - Compute the coarse-level right-hand side (FAS scheme [36, Sec. 5.3]) :

$$\mathbf{S}_{n-1} = \mathbf{I}_n^{n-1}\left(\mathbf{S}_n - \mathbf{N}_n(\bar{\boldsymbol{\phi}}_n)\right) + \mathbf{N}_{n-1}\left(\mathbf{I}_n^{n-1}\bar{\boldsymbol{\phi}}_n\right) \tag{6.12}$$

- Compute an approximate solution $\hat{\boldsymbol{\psi}}_{n-1}$ of the following coarse grid equation:

$$\mathbf{N}_{n-1}(\boldsymbol{\psi}_{n-1}) = \mathbf{S}_{n-1}. \tag{6.13}$$

  – If $n = n_{\min} + 1$ employ λ smoothing steps:

$$\hat{\boldsymbol{\psi}}_{n_{\min}} = \text{Smooth}\left(\lambda, \bar{\boldsymbol{\phi}}_{n_{\min}}, \mathbf{N}_{n_{\min}}, \mathbf{S}_{n_{\min}}\right). \tag{6.14}$$

  – If $n > n_{\min} + 1$ get an approximate solution to Eq. (6.13) using $\bar{\boldsymbol{\phi}}_{n-1}$ as initial guess:

$$\hat{\boldsymbol{\psi}}_{n-1} = \text{FASVcycle}\left(n-1, \bar{\boldsymbol{\phi}}_{n-1}, \mathbf{N}_{n-1}, \mathbf{S}_{n-1}, \lambda\right) \tag{6.15}$$

- Compute the coarse-grid correction:

$$\hat{\boldsymbol{\varphi}}_{n-1} = \hat{\boldsymbol{\psi}}_{n-1} - \bar{\boldsymbol{\phi}}_{n-1}. \tag{6.16}$$

- Compute the coarse-grid-corrected approximation at level n:

$$\boldsymbol{\phi}_n^{\text{CGC}} = \mathbf{I}_{n-1}^{n} \hat{\boldsymbol{\varphi}}_{n-1} + \bar{\boldsymbol{\phi}}_n. \tag{6.17}$$

3. Post-smoothing:

- Compute $\boldsymbol{\phi}_n^{k+1,m+1}$ by applying λ smoothing steps:

$$\boldsymbol{\phi}_n^{k+1,m+1} = \text{Smooth}\left(\lambda, \boldsymbol{\phi}_n^{\text{CGC}}, \mathbf{N}_n, \mathbf{S}_n\right) \tag{6.18}$$

Another important thing to notice is the calculation of source $\mathbf{S}$. By definition $[\cdot \star \cdot]$ is an expensive summation. However, by the property of periodic convolution we can apply discrete Fourier transform (DFT) to accelerate the speed. Lets denote that $\widehat{\phi^k}$ and $\widehat{J}$ stands for the DFT image of ϕ^k and J. By the property of DFT the numerical convolution is nothing but the point-wise product of $\widehat{\phi^k}$ and $\widehat{J}$. Also due to the periodic boundary condition and the special order in fast Fourier transform (FFT) schemes, $\widehat{J}$ needs to be shifted. Thus $[\widehat{J \star \phi^k}]_{i,j} = \widehat{J}^s_{i,j} \times \widehat{\phi^k}_{i,j}$ where $\widehat{J}^s$ is the shifted DFT image of J. Noticing that the potential J is independent of ϕ^k and $\tilde{w}^k$, thus we could compute and shift $\widehat{J}$ in the beginning and store it for later use. Overall when we compute $\mathbf{S}_{n_{\max}}\left(\boldsymbol{\phi}^k_{n_{\max}}\right)$, this is what we should do:

- Compute $S^{(1)}_{i,j}\left(\boldsymbol{\phi}^k\right) = \phi^k_{i,j}$.
- Use FFT to compute $\widehat{\phi^k}$.
- Compute $[\widehat{J \star \phi^k}]_{i,j}$ by $\widehat{J}^s_{i,j} \times \widehat{\phi^k}_{i,j}$.
- Use inverse FFT to compute $\left[J \star \phi^k\right]_{i,j}$.
- Compute $S^{(2)}_{i,j}\left(\boldsymbol{\phi}^k\right) = -([J_c \star 1] + [J_e \star 1] + \gamma_e)\phi^k_{i,j} - \left[J \star \phi^k\right]_{i,j}$.

The combined algorithm for time stepping using the FAS V-Cycle multigrid scheme as the iterative solver is given in the following algorithm:

Combined Time Stepping and FAS V-Cycle Iteration Algorithm

initialize $\boldsymbol{\phi}^{k=0}_{n_{\max}}$ and $\widehat{J}^s$

Time Step Loop: **for** $k = 0,\ k_{\max} - 1$

  set $\boldsymbol{\phi}^{k+1,m=0}_{n_{\max}} = \boldsymbol{\phi}^k_{n_{\max}}$

  calculate $\mathbf{S}_{n_{\max}}\left(\boldsymbol{\phi}^k_{n_{\max}}\right)$

  V-cycle Loop: **for** $m = 0,\ m_{\max} - 1$

    $\boldsymbol{\phi}^{k+1,m+1}_{n_{\max}} = \text{FASVcycle}\left(n_{\max}, \boldsymbol{\phi}^{k+1,m}_{n_{\max}}, \mathbf{N}_{n_{\max}}, \mathbf{S}_{n_{\max}}, \lambda\right)$

    if $\left\|\mathbf{S}_{n_{\max}}\left(\boldsymbol{\phi}^k_{n_{\max}}\right) - \mathbf{N}_{n_{\max}}\left(\boldsymbol{\phi}^{k+1,m+1}_{n_{\max}}\right)\right\|_{2,\star} < \tau$ **then**

      set $\boldsymbol{\phi}^{k+1}_{n_{\max}} = \boldsymbol{\phi}^{k+1,m+1}_{n_{\max}}$ and **exit** V-cycle Loop

  end for V-cycle Loop

end for Time Step Loop

The parameter $\tau > 0$ is the stopping tolerance. The scaled 2-norm in algorithm is defined via

$$\|\mathbf{R}(\boldsymbol{\phi})\|_{2,\star} := \sqrt{\frac{h^2}{3L_xL_y}\sum_{k=1}^{3}\sum_{i=1}^{m}\sum_{j=1}^{n}\left(R_{i,j}^{(k)}(\boldsymbol{\phi})\right)^2}, \tag{6.19}$$

where $\mathbf{R}(\boldsymbol{\phi}) := \mathbf{S}\left(\phi^k\right) - \mathbf{N}(\boldsymbol{\phi})$ is the $2 \times m \times n$ residual array, and $R_{i,j}^{(k)}(\boldsymbol{\phi})$ are its components.

6.3 The Numerical Convergence Test

In this section we verify the convergence rate of schemes through numerical tests. Since we don't have the exact solution to compare, we use the difference between simulations on coarse and finer grids with same initial condition and ending time. Difference e_A is evaluated by the average value of function on fine grid and we use the discrete L^2 norm.

6.3.1 First Order Scheme for nCH Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-0.5, 0.5]^2$.
- The initial condition is a smooth function $0.5\sin(2\pi x_1)\sin(2\pi x_2)$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.20}$$

  where $\sigma_1 = 0.05$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

- $\gamma_e = 1$, $\gamma_c = 0$.

Table 6.1: The Difference between Coarse and Fine Grids

coarse h	fine h	$\|e_A\|_2$	rate
1/128	1/256	0.002143162029982	–
1/256	1/512	0.000607406265800	1.8190
1/512	1/1024	0.000157056139044	1.9514
1/1024	1/2048	0.000039602788901	1.9876

- The time step dt and the grid size h satisfies $dt = h^2$.
- In all cases, the ending time is 0.002441406250000.

The numerical result of this experiment is shown in Tab. 6.1 and Fig. 6.1

6.3.2 First Order Scheme for nAC Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-0.5, 0.5]^2$.
- The initial condition is a smooth function $0.5\sin(2\pi x_1)\sin(2\pi x_2)$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.21}$$

  where $\sigma_1 = 0.05$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

- $\gamma_e = 1$, $\gamma_c = 0$.
- The time step dt and the grid size h satisfies $dt = h^2$.
- In all cases, the ending time is 0.002441406250000.

The numerical result of this experiment is shown in Tab. 6.2 and Fig. 6.2

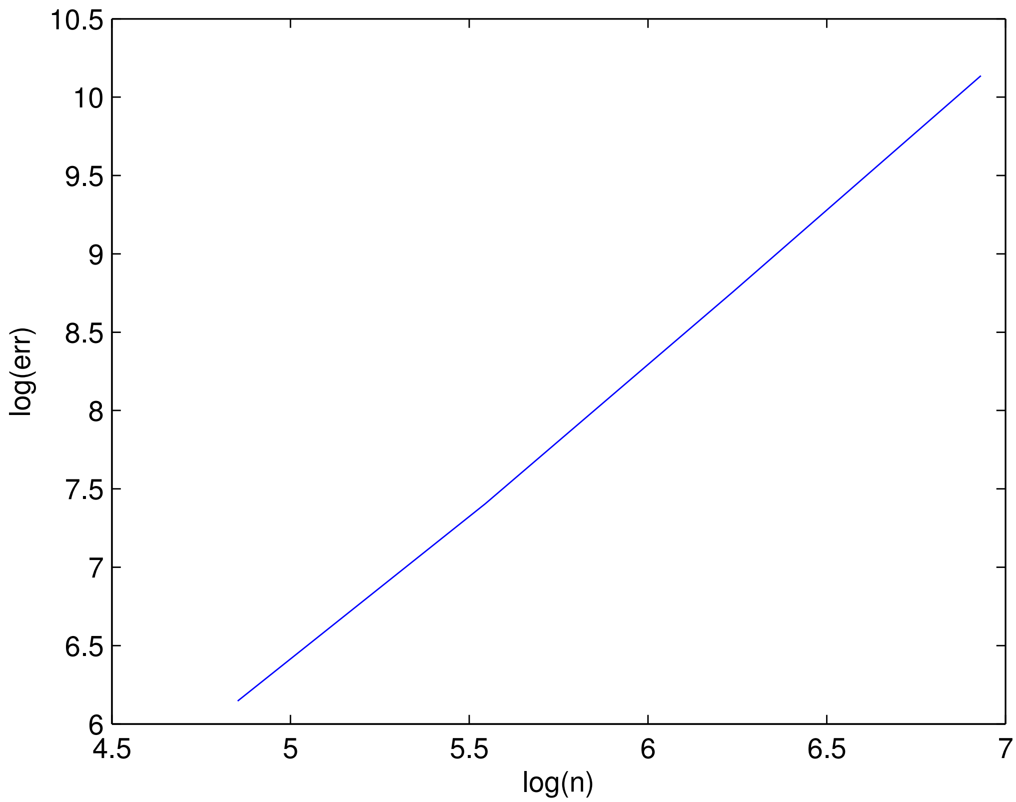


Figure 6.1: The log − log plot of Tab. 6.1. The slope is around 1.9.

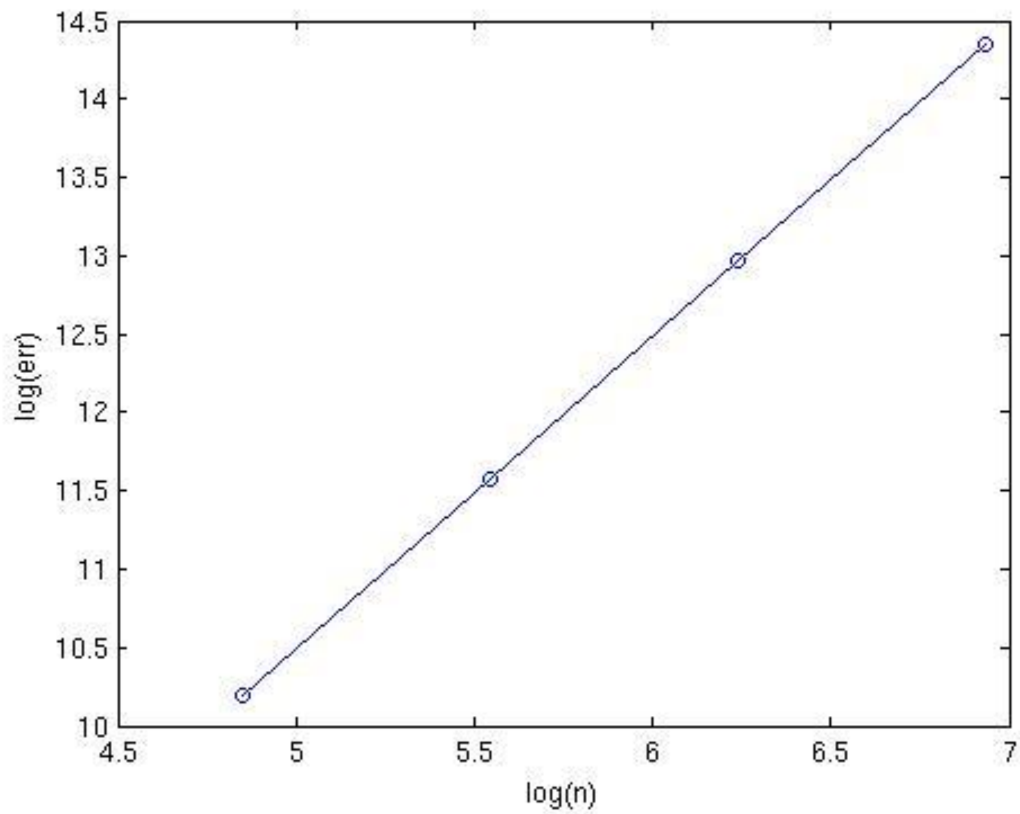


Figure 6.2: The log − log plot of Tab. 6.2. The slope is around 1.9.

Table 6.2: The Difference between Coarse and Fine Grids

coarse h	fine h	$\|e_A\|_2$	rate
1/128	1/256	3.757601789300150e-05	–
1/256	1/512	9.394347142961551e-06	1.999947375064814
1/512	1/1024	2.348608223302800e-06	1.999986831347253
1/1024	1/2048	5.871533921806258e-07	1.999996716437571

6.3.3 Second Order Scheme for nCH Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-0.5, 0.5]^2$.
- The initial condition is a smooth function $0.5\sin(2\pi x_1)\sin(2\pi x_2)$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.22}$$

  where $\sigma_1 = 0.05$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.
- $\gamma_e = 1$, $\gamma_c = 0$.
- The time step dt and the grid size h satisfies $dt = h$.
- In all cases, the ending time is 0.0015625.

The numerical result of this experiment is shown in Tab. 6.3 and Fig. 6.3

Table 6.3: The Difference between Coarse and Fine Grids (Conserved Dynamics)

coarse h	fine h	$\|e_A\|_2$	rate
1/64	1/128	0.023594977666378	–
1/128	1/256	0.003642747274851	2.695380992993224
1/256	1/512	8.669302357639438e-04	2.071039102165462
1/512	1/1024	2.162606042972027e-04	2.003145023762793
1/1024	1/2048	5.411334233516024e-05	1.998714618858811

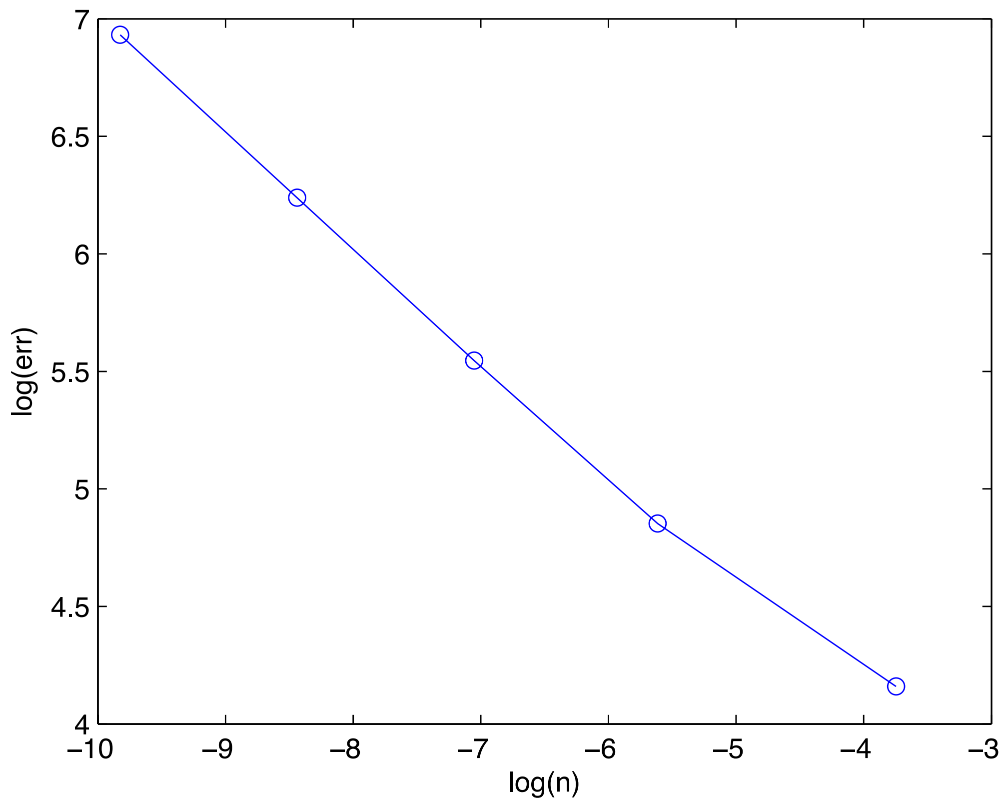


Figure 6.3: The $\log - \log$ plot of Tab. 6.3. The slope is around 2.

6.3.4 Second Order Scheme for nAC Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-0.5, 0.5]^2$.
- The initial condition is a smooth function $0.5\sin(2\pi x_1)\sin(2\pi x_2)$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.23}$$

  where $\sigma_1 = 0.05$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

- $\gamma_e = 1$, $\gamma_c = 0$.
- The time step dt and the grid size h satisfies $dt = h$.
- In all cases, the ending time is 0.0015625.

The numerical result of this experiment is shown in Tab. 6.4 and Fig. 6.4

Table 6.4: The Difference between Coarse and Fine Grids (Non conserved Dynamics)

coarse h	fine h	$\|e_A\|_2$	rate
1/64	1/128	1.510704455248701e-04	–
1/128	1/256	3.777326690535997e-05	1.9997839793014266
1/256	1/512	9.443660642523572e-06	1.999947459441191
1/512	1/1024	2.360936173440859e-06	1.999987159664891
1/1024	1/2048	5.902355596047761e-07	1.999996293884224

6.4 The Energy Decay Test

In this section we are going to verify the formation of spinodal decomposition with the random initial condition, *i.e.*, the random perturbation over a constant. The corresponding energy decay is also verified.

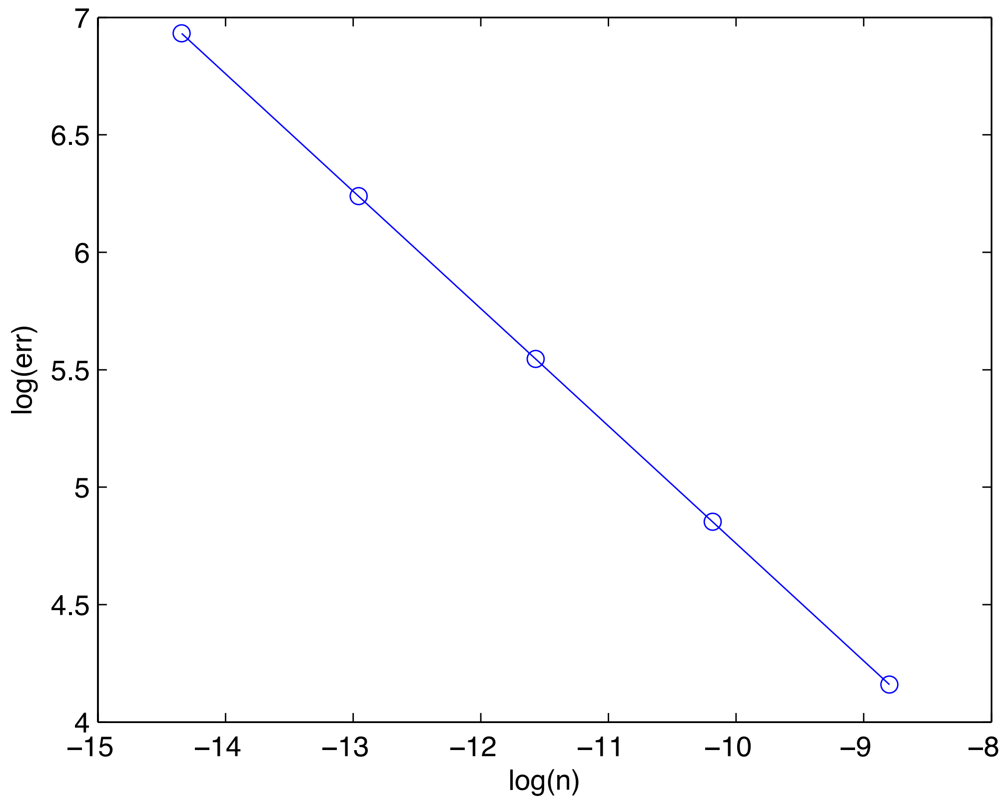


Figure 6.4: The log − log plot of Tab. 6.4. The slope is around 2.

6.4.1 First Order Scheme for nCH Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-5, 5]^2$.
- The initial condition is the random perturbation over a constant and the initial average is $\phi_{ave} = 0$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.24}$$

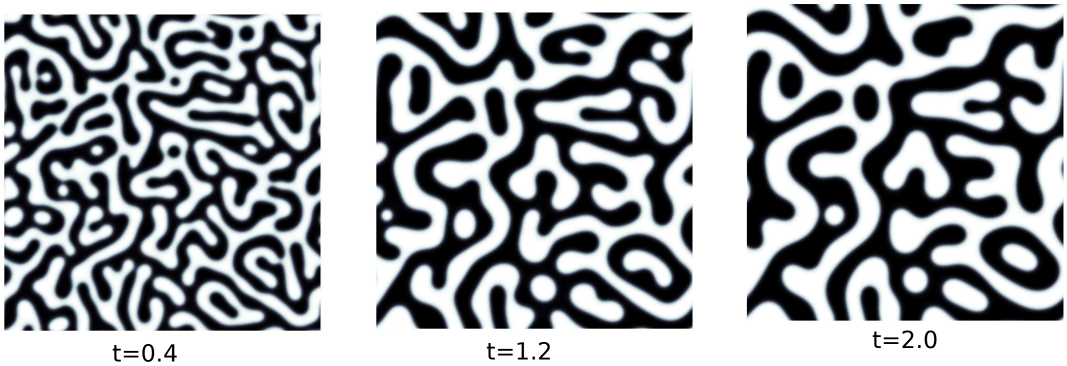


Figure 6.5: Spinodal Decomposition of Random Initial Condition by 1st Order Scheme

where $\sigma_1 = 0.05$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

- $\gamma_e = 1$, $\gamma_c = 0$.

The numerical result of this experiment is shown in Fig. 6.5 and Fig. 6.6

6.4.2 First Order Scheme for nAC Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-0.5, 0.5]^2$.
- The initial condition is the random perturbation over a constant and the initial average is $\phi_{ave} = 0$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.25}$$

where $\sigma_1 = 0.05$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

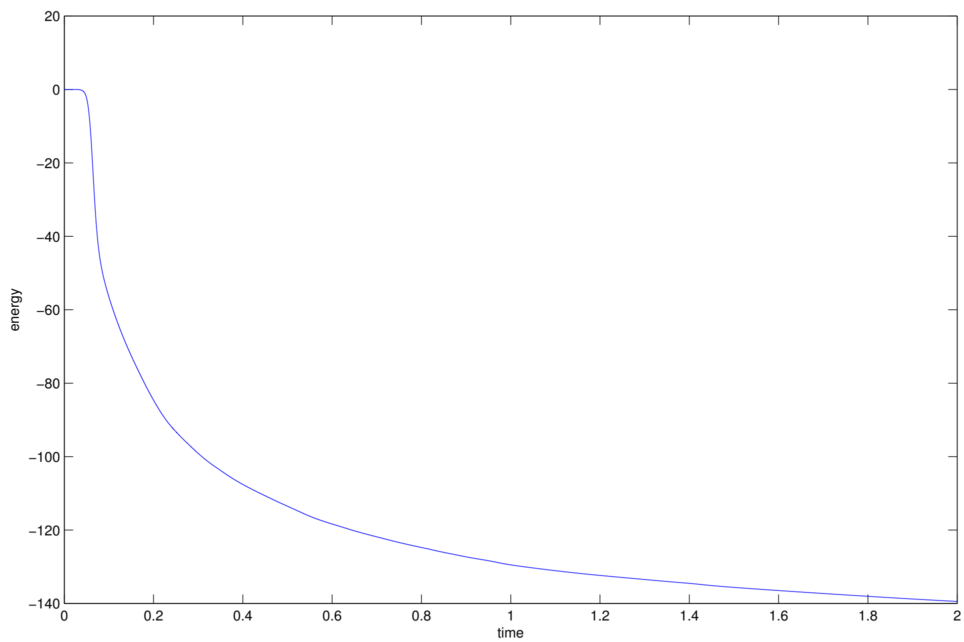


Figure 6.6: Decreasing of Energy for the simulation shown in Fig. 6.5

- $\gamma_e = 1$, $\gamma_c = 0$.

The numerical result of this experiment is shown in Fig. 6.7 and Fig. 6.8

6.4.3 Second Order Scheme for nCH Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-0.5, 0.5]^2$.
- The initial condition is the random perturbation over a constant and the initial average is $\phi_{ave} = 0$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.26}$$

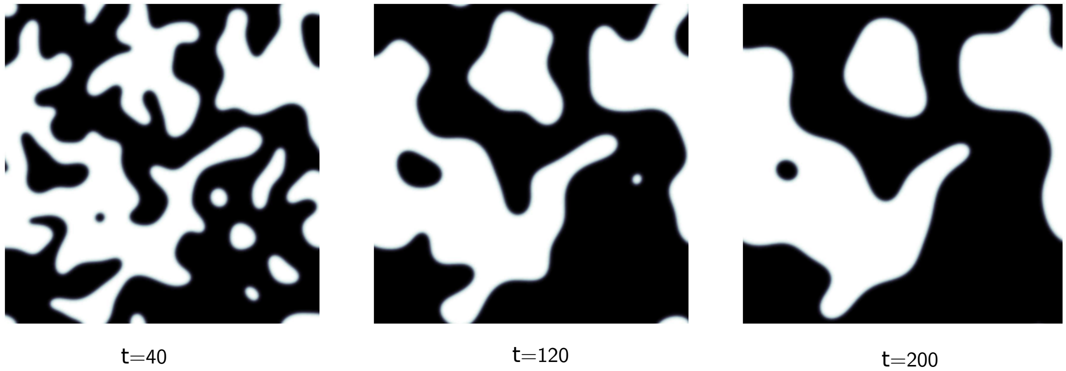


Figure 6.7: Spinodal Decomposition of Random Initial Condition by 1st Order Scheme

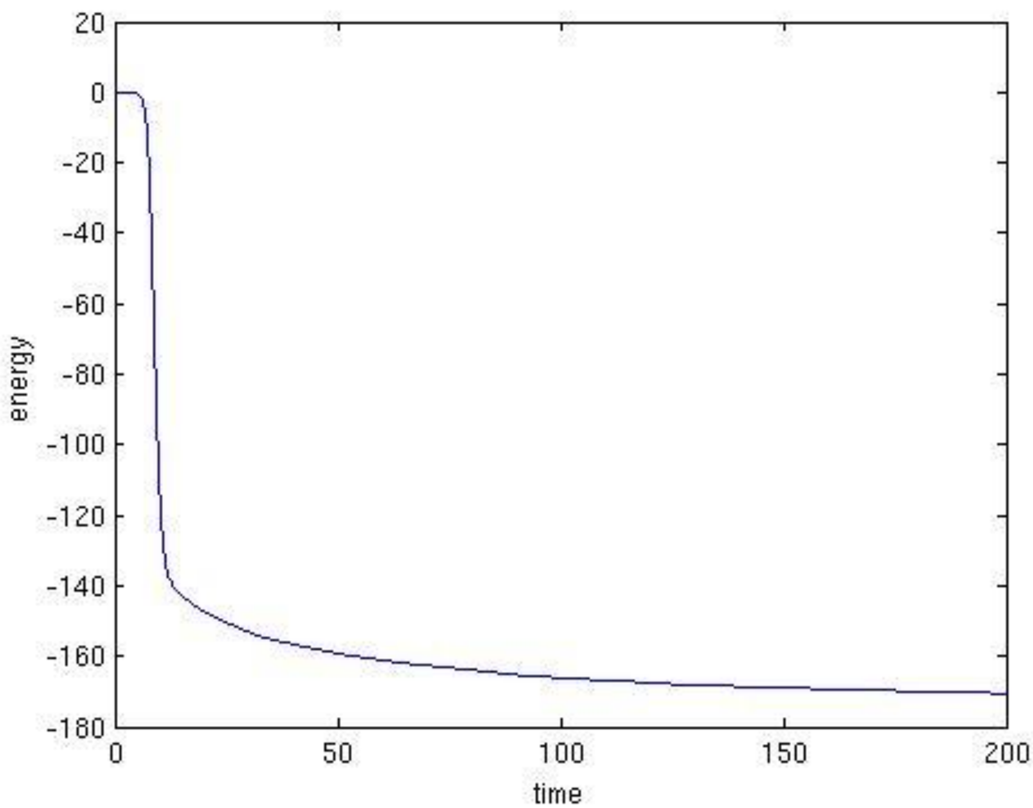


Figure 6.8: Decreasing of Energy for the simulation shown in Fig. 6.7

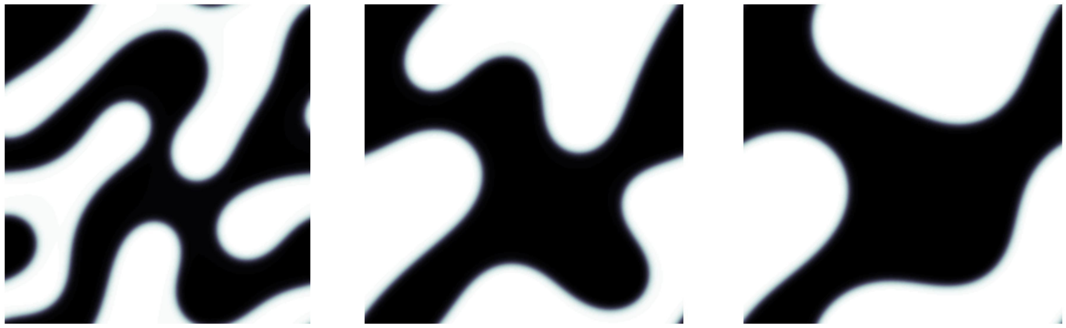


Figure 6.9: Spinodal Decomposition of Random Initial Condition by 1st Order Scheme

where $\sigma_1 = 0.1$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

- $\gamma_e = 1$, $\gamma_c = 0$.

The numerical result of this experiment is shown in Fig. 6.9 and Fig. 6.10

6.4.4 Second Order Scheme for nAC Equation

Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-0.5, 0.5]^2$.
- The initial condition is the random perturbation over a constant and the initial average is $\phi_{ave} = 0$.
- J is a positive Gaussian function defined as

$$J = \alpha \exp\left(-\frac{x_1^2 + x_2^2}{\sigma_1^2}\right) \tag{6.27}$$

where $\sigma_1 = 0.1$ and $\alpha = \frac{1}{\sigma_1^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

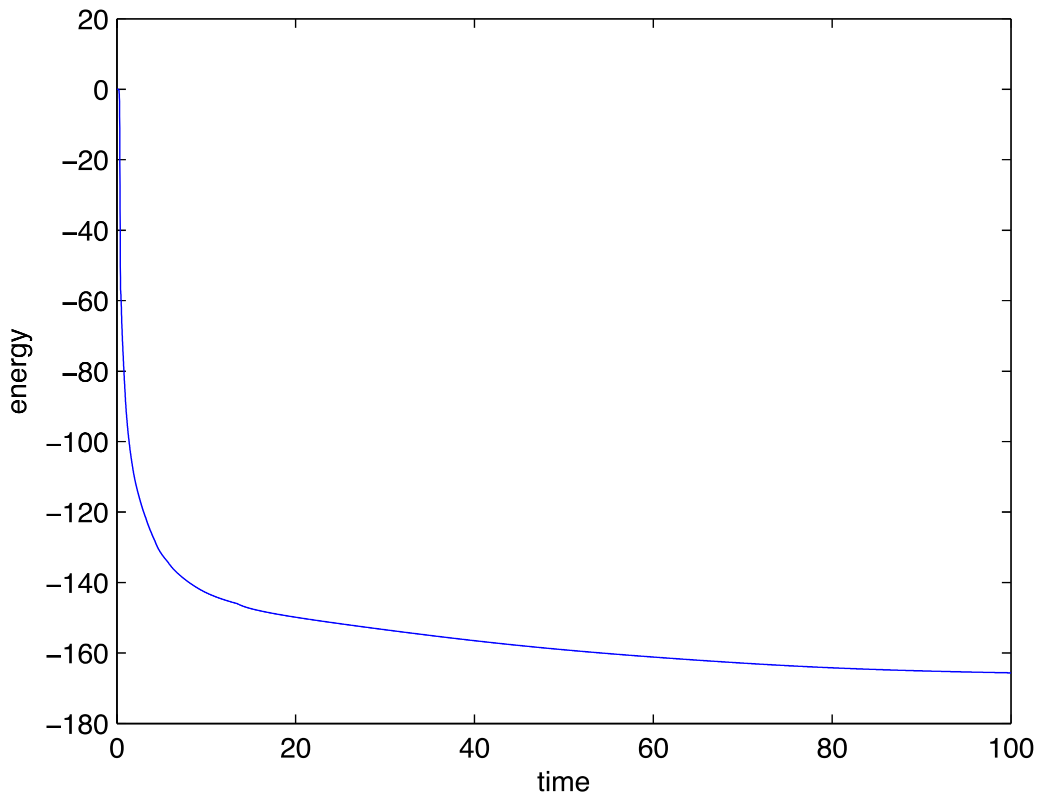


Figure 6.10: Decreasing of Energy for the simulation shown in Fig. 6.9

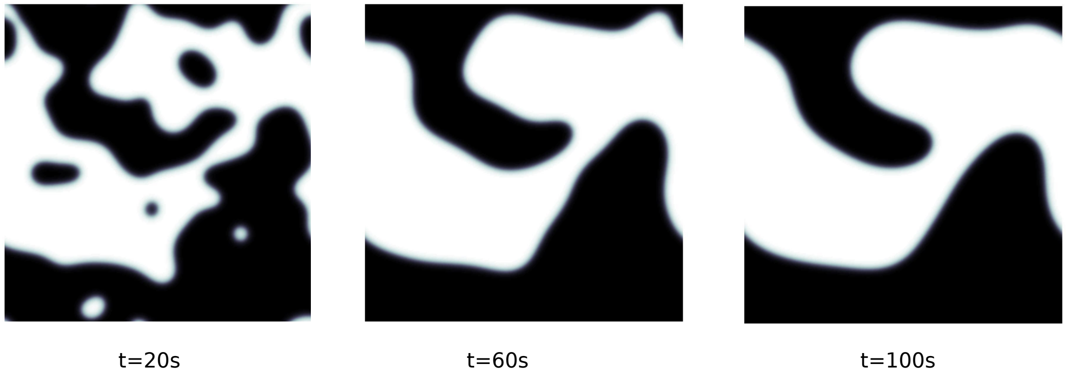


Figure 6.11: Spinodal Decomposition of Random Initial Condition by 1st Order Scheme

- $\gamma_e = 1$, $\gamma_c = 0$.

The numerical result of this experiment is shown in Fig. 6.11 and Fig. 6.12

6.5 Nucleation Phenomena for nCH Equation

In this section we discuss nucleation phenomena in the nCH equation. In Sec. 1.5 we already discussed the similarity between RAnCH equation and PFC equation, and the later is widely known for its simulation of nucleation. First we are going to reproduce the nucleation phenomena with RAnCH equation and verify its reliability by showing the decreasing of energy. Next we discuss two factors which have strong influence on nucleation. In the last part we discuss the unique phenomena which shows that nucleation can be influenced by the shape of anisotropic potentials.

6.5.1 Nucleation Phenomena

In this section we discuss results of numerical experiments for nCH, which resemble the pattern similar to the phase field crystal equations shown in [25]. Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-10, 10]^2$.

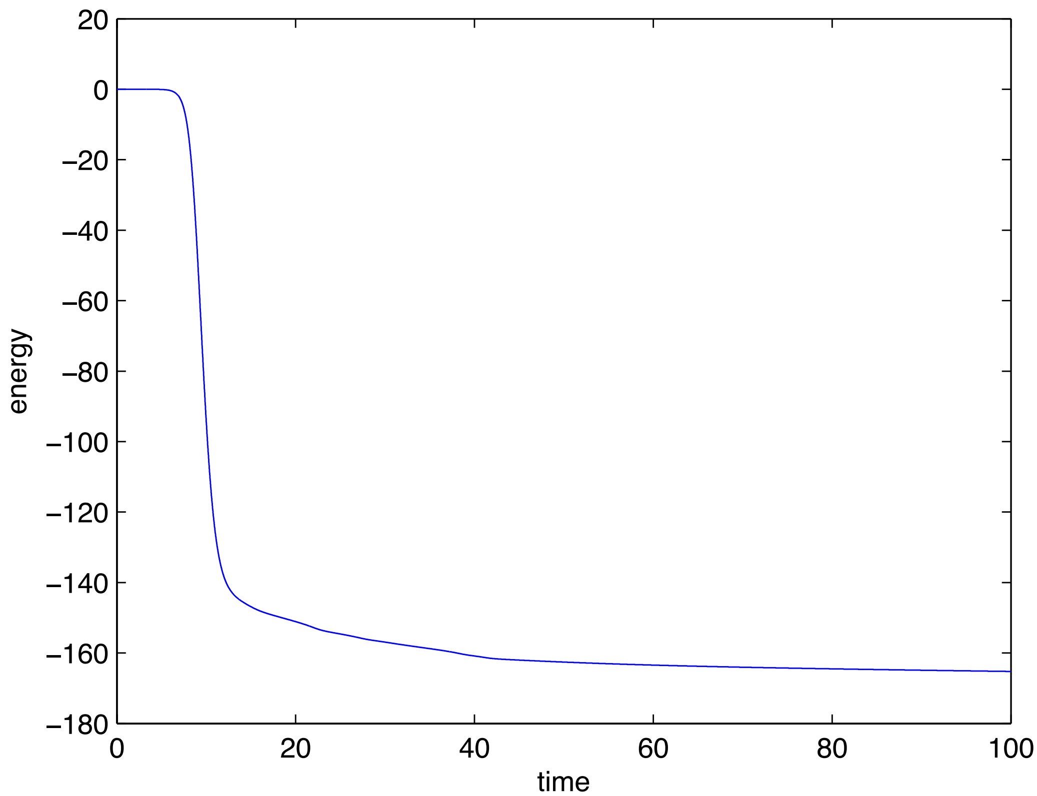


Figure 6.12: Decreasing of Energy for the simulation shown in Fig. 6.11

- The initial condition is the random perturbation over a constant and the average of ϕ is $\phi_{ave} = 0.07$.

- J is a positive Gaussian function defined as

$$J = \alpha e^{-\frac{x^2}{\sigma_1^2}} - \beta e^{-\frac{x^2}{\sigma_2^2}} \tag{6.28}$$

  where $\sigma_1 = 0.08$, $\sigma_2 = 0.2$, $\alpha = \frac{0.1}{\sigma_1^2}$ and $\beta = \frac{0.05}{\sigma_2^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

- $\gamma_e = 0$, $\gamma_c = 0.01$.

The numerical result is shown in following figures: Fig. 6.13 shows nucleation; Fig. 6.14 shows the shape of J; Fig. 6.15 verifies the corresponding energy decay.

Remark 6.5.1. *The potential J in this experiment is motivated by the phase field equation in [25]. The Fourier image of J is similar to the Fourier image of gradient part in the phase field equation.*

With the small modification of the initial condition, we can also simulate the growth of nucleation. Fig. 6.16 shows nucleation with the random initial perturbation in one block. Fig. 6.17 shows nucleation with the random initial perturbation in four blocks.

6.5.2 The Phase Diagram of Nucleation

In this section we discuss factors which influence nucleation. In many previous physics literature it is shown that the average of ϕ is crucial (see [22, 15]). It is also clear that the size of the linear coefficient $\gamma_c - \gamma_e$ is another influential factor. Here the setting of the experiment satisfies the following requirements:

- We use a square domain $\Omega = [-10, 10]^2$.

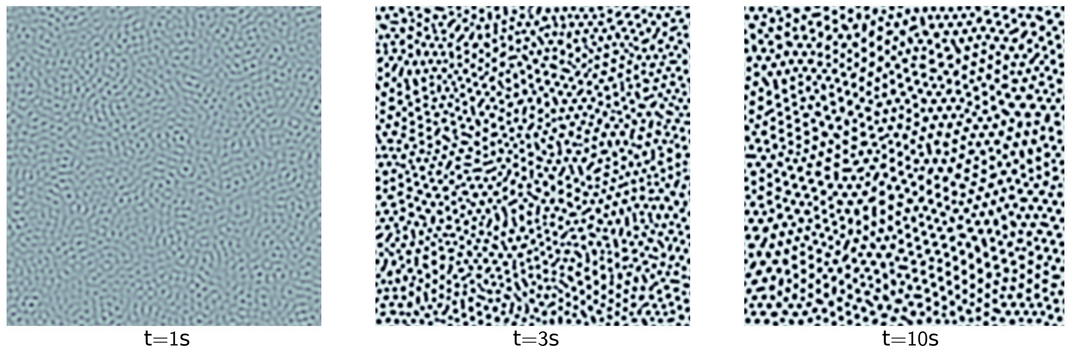


Figure 6.13: The nucleation for nCH with the random initial condition.

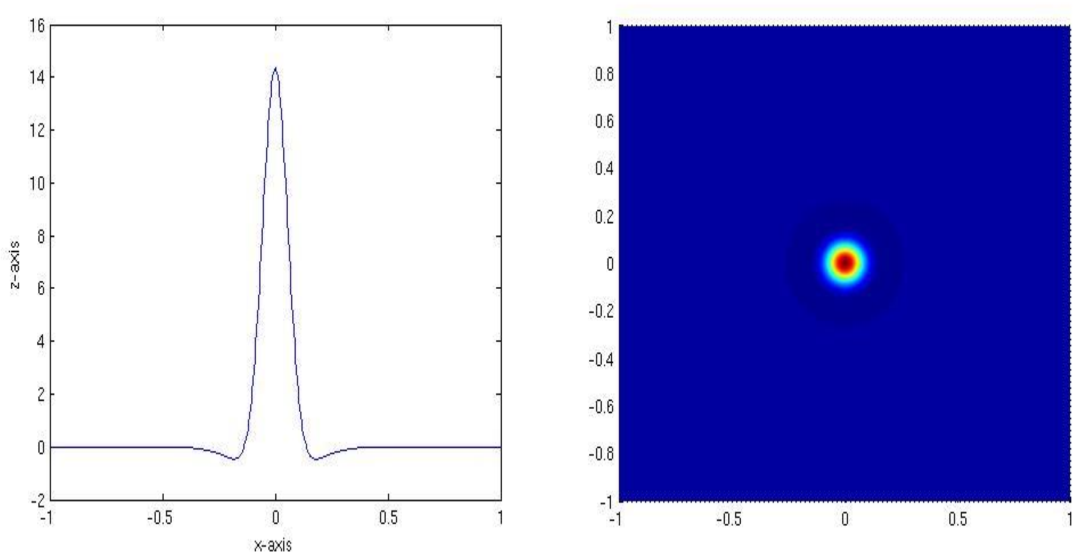


Figure 6.14: The potential for the simulation in Fig. 6.13. The right figure is the view from top. The left figure is a cut view for $y = 0$.

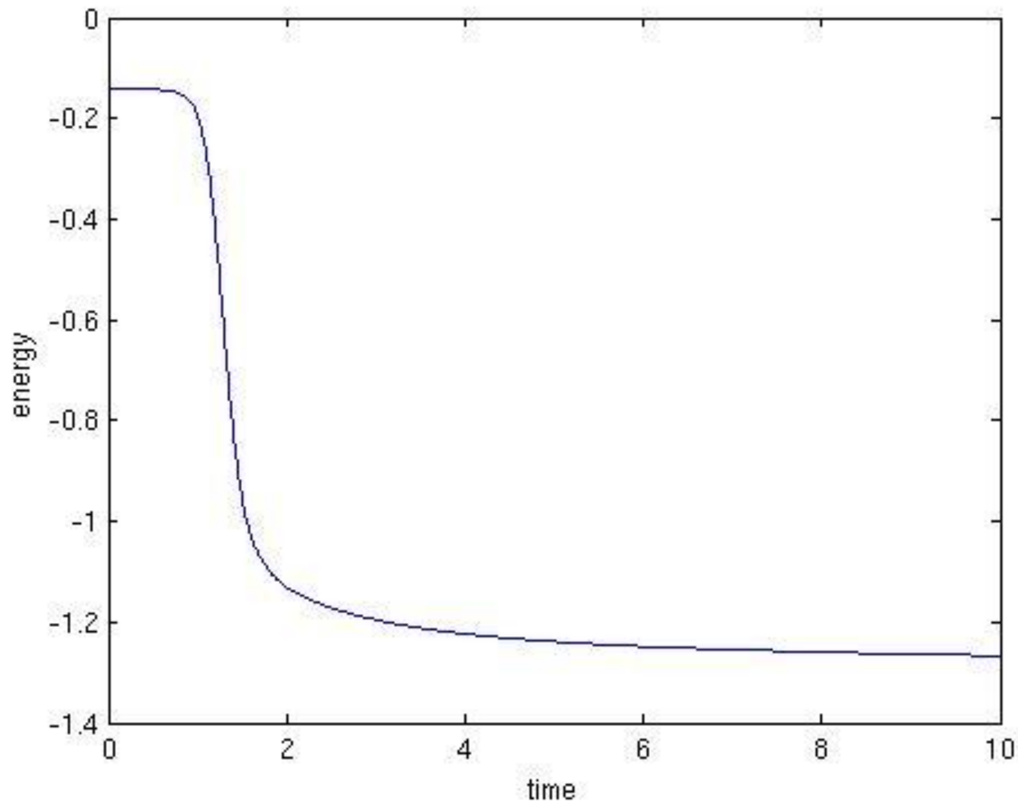


Figure 6.15: The corresponding energy for nucleation shown in Fig. 6.13.

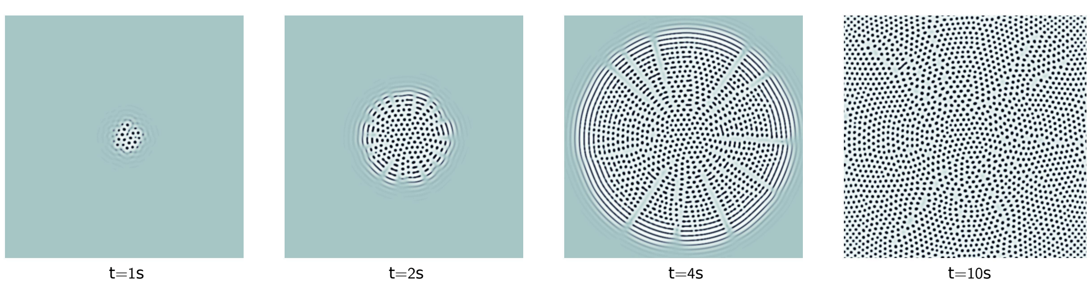


Figure 6.16: The crystal growth with the random initial perturbation in a small block. J is defined as Fig. 6.14.

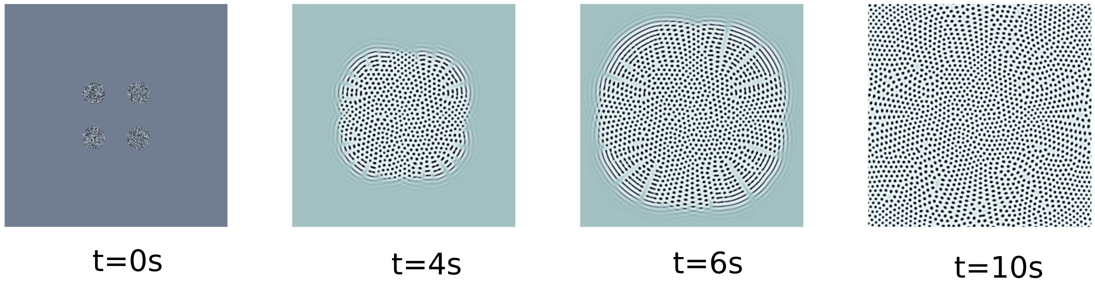


Figure 6.17: The crystal growth with the random initial perturbation in four small blocks. J is defined as Fig. 6.14.

- The initial condition is the random perturbation over a constant and the average of ϕ is a parameter.
- J is a positive Gaussian function defined as

$$J = \alpha e^{-\frac{x^2}{\sigma_1^2}} - \beta e^{-\frac{x^2}{\sigma_2^2}} \tag{6.29}$$

  where $\sigma_1 = 0.08$, $\sigma_2 = 0.2$, $\alpha = \frac{0.1}{\sigma_1^2}$ and $\beta = \frac{0.05}{\sigma_2^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.

- The value of $\gamma_c - \gamma_e$ is another parameter.

Fig. 6.18 is a phase diagram verifying such phenomena.

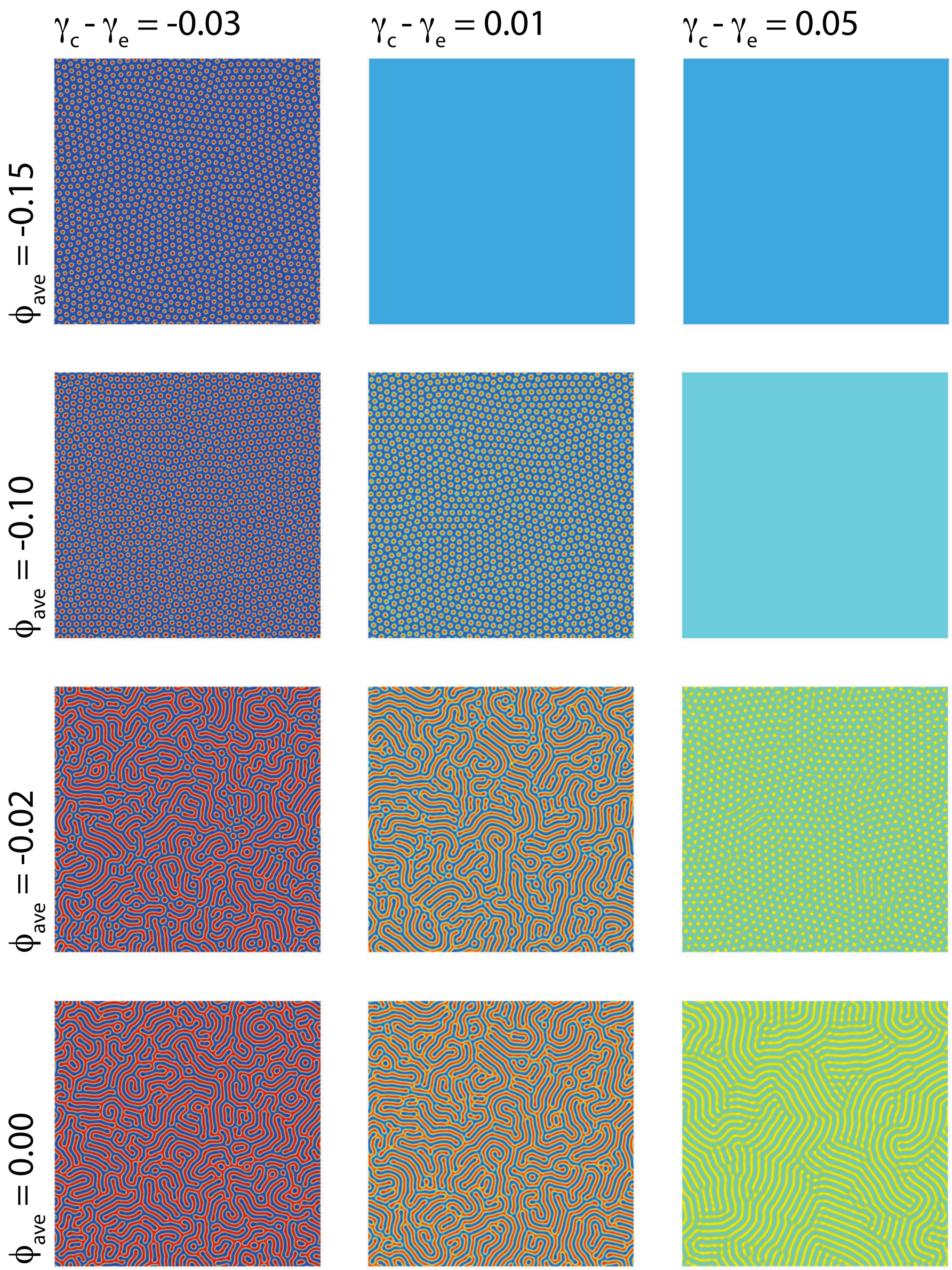


Figure 6.18: The phase diagram for nucleation at same time.

6.5.3 Controlling the Nucleation

In this section we discuss the influence of the shape of J to nucleation. First of all let's denote three even convolution potentials J_1, J_2 and J_3 defined as:

$$J_1 = \alpha \exp\left(-\frac{x_1^2+x_2^2}{\sigma_1^2}\right) - \beta \exp\left(-\frac{x_1^2+x_2^2}{\sigma_2^2}\right) , \tag{6.30}$$

$$\begin{aligned} J_2 =& 0.5\alpha \left[\exp\left(-\frac{x_1^2}{(0.5\sigma_1)^2} - \frac{x_2^2}{\sigma_1^2}\right) + \exp\left(-\frac{x_1^2}{\sigma_1^2} - \frac{x_2^2}{(0.5\sigma_1)^2}\right)\right] \\ & - 0.5\beta \left[\exp\left(-\frac{x_1^2}{(0.5\sigma_2)^2} - \frac{x_2^2}{\sigma_2^2}\right) + \exp\left(-\frac{x_1^2}{\sigma_2^2} - \frac{x_2^2}{(0.5\sigma_2)^2}\right)\right] , \end{aligned} \tag{6.31}$$

$$\begin{aligned} J_3 =& 0.5\alpha \exp\left(-\frac{0.5(x_1-x_2)^2}{(0.5\sigma_1)^2} - \frac{0.5(x_1+x_2)^2}{\sigma_1^2}\right) \\ & + 0.5\alpha \exp\left(-\frac{0.5(x_1-x_2)^2}{\sigma_1^2} - \frac{0.5(x_1+x_2)^2}{(0.5\sigma_1)^2}\right) \\ & - 0.5\beta \exp\left(-\frac{0.5(x_1-x_2)^2}{(0.5\sigma_2)^2} - \frac{0.5(x_1+x_2)^2}{\sigma_2^2}\right) \\ & - 0.5\beta \exp\left(-\frac{0.5(x_1-x_2)^2}{\sigma_2^2} - \frac{0.5(x_1+x_2)^2}{(0.5\sigma_2)^2}\right) . \end{aligned} \tag{6.32}$$

Figs. 6.19, 6.20 and 6.21 present the shape of J_1, J_2 and J_3. As these figures shown, the shape of these three potentials have different decay speed over different directions.

The setting of all experiments in this section satisfies the following requirements:

- We use a square domain $\Omega = [-10, 10]^2$.
- The initial condition is the random perturbation over a constant and the average of ϕ is $\phi_{ave} = 0.2$.
- The value of parameters for J_1, J_2 and J_3 are $\sigma_1 = 0.08$, $\sigma_2 = 0.2$, $\alpha = \frac{0.1}{\sigma_1^2}$ and $\beta = \frac{0.08}{\sigma_2^2}$. By this setting J has the sufficient decaying speed on Ω, therefore it can be viewed as periodic.
- The value of $\gamma_c - \gamma_e$ is 0.

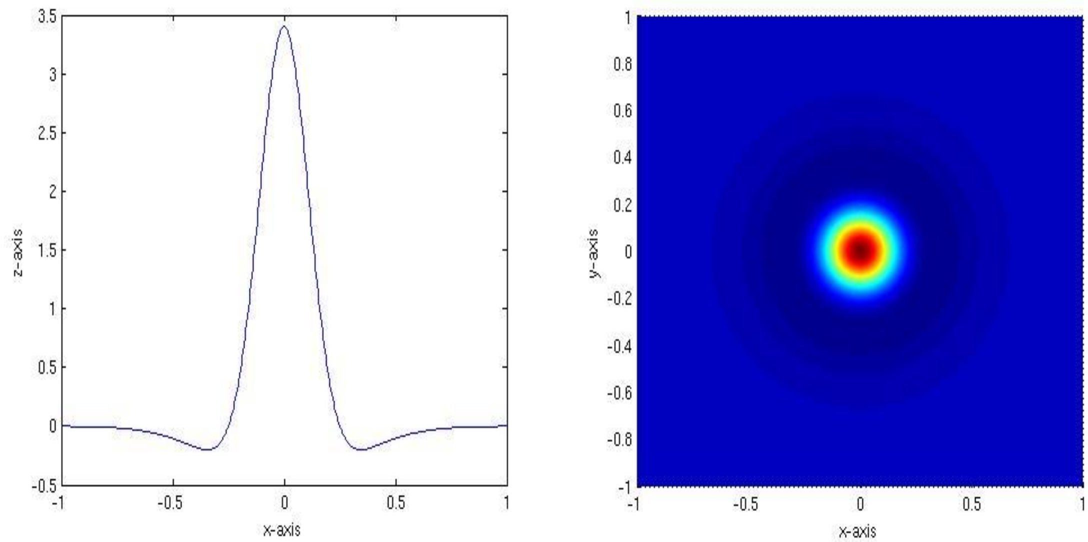


Figure 6.19: The figure of potential J_1.

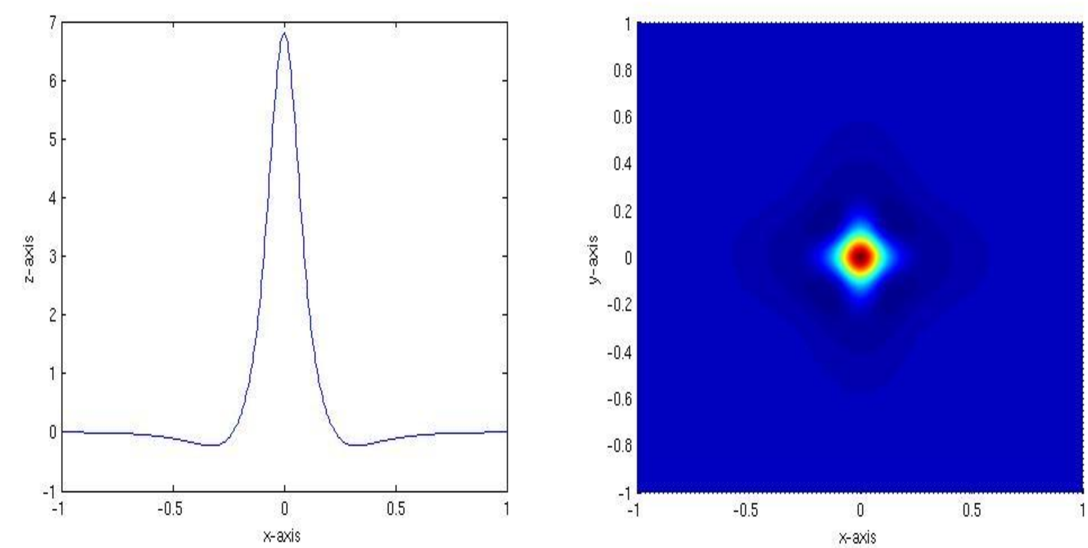


Figure 6.20: The figure of potential J_2.

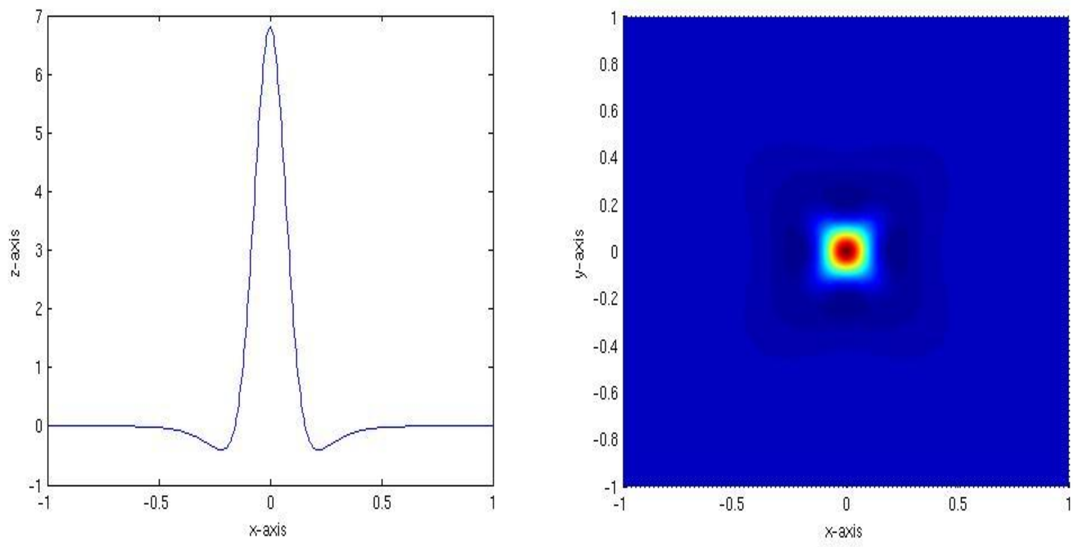


Figure 6.21: The figure of potential J_3.

Figs. 6.22 and 6.23 indicate the difference of nucleation by different potentials. These comparisons indicate that the shape of the potential will have a strong influence on the formulation of nucleation.

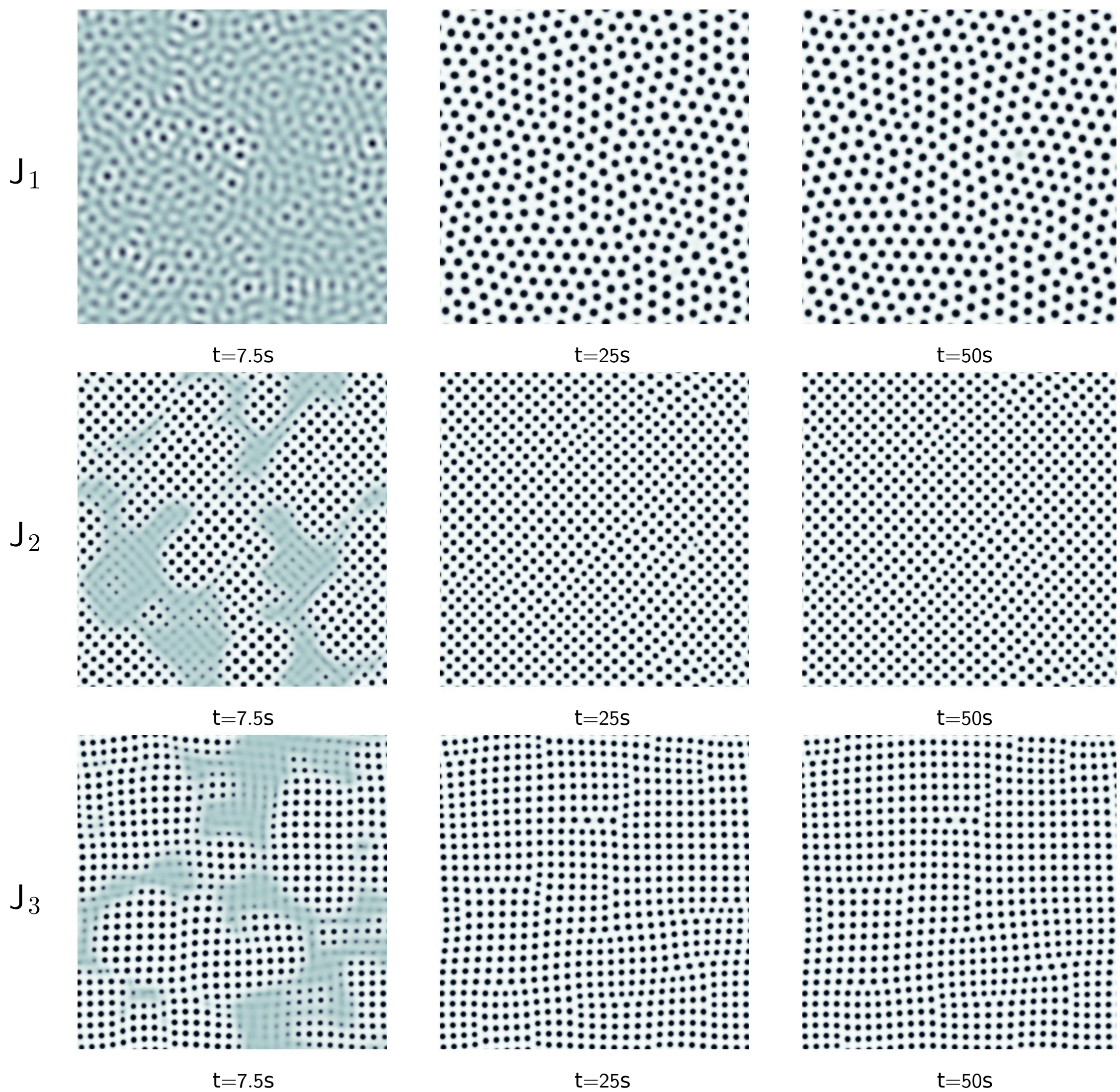


Figure 6.22: The comparison of nucleation with random initial condition.

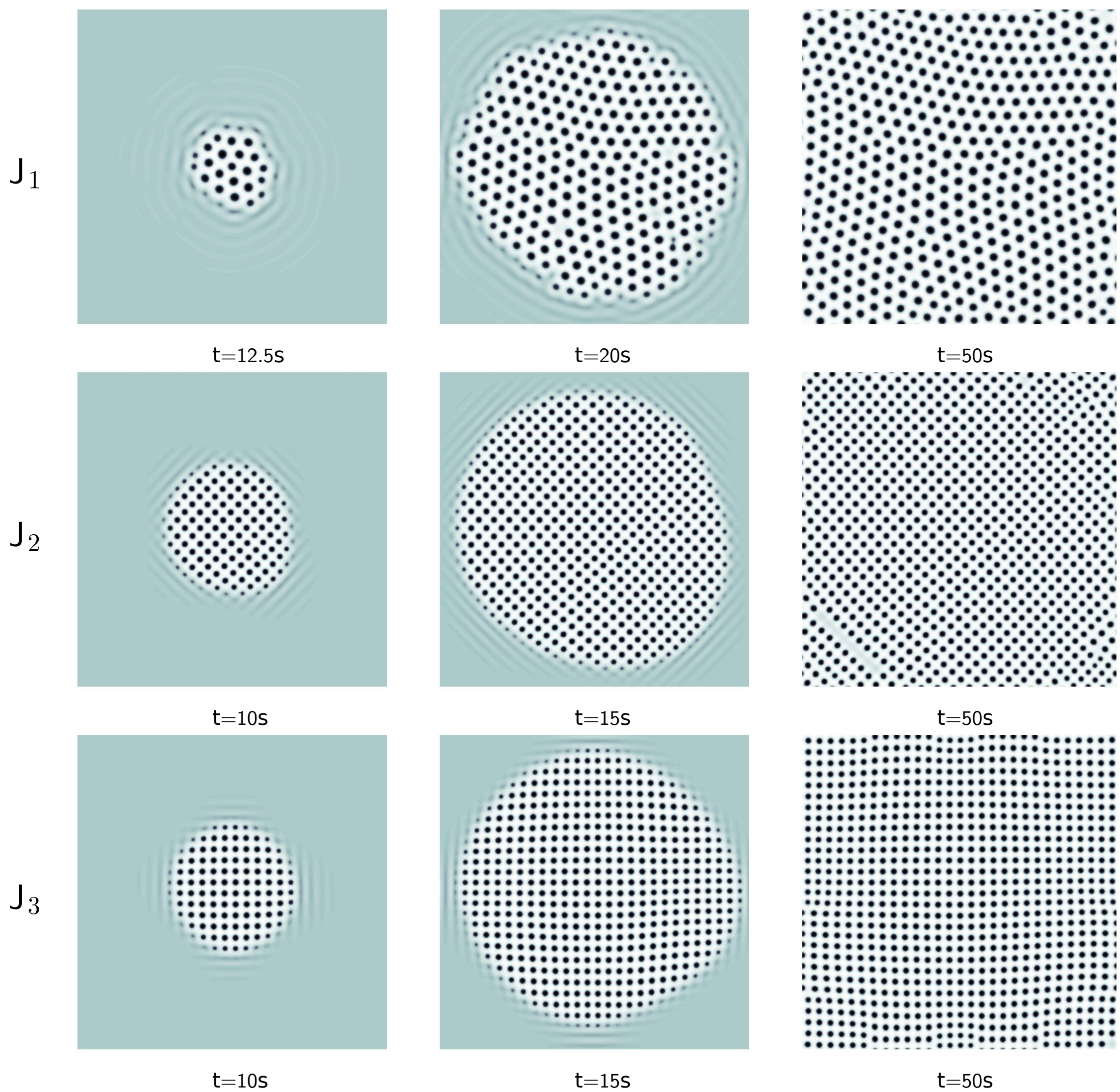


Figure 6.23: The comparison of nucleation with one block of perturbation.

Chapter 7

Conclusion

7.1 Concluding Remark

In this dissertation we derived the first and second order in time, second order in space, unconditionally energy stable schemes for nCH and nAC equations. We analyzed these schemes in details, proving the energy stability and unique solvability. Also we proved convergence of the scheme for most of them. The numerical result was also presented to verify these results.

Another major contribution in this dissertation is that we derived a highly efficient stable multi-grid solver based on schemes we proposed. The details of the solver is given. With this powerful solver we managed to produce the third main contribution: simulations of nucleation phenomena. Also we analyzed the influence of anisotropic potential. This is the first result in this field, and it has huge practical value.

7.2 Future Work

Our immediate plan is to apply this scheme to many applications of DDFT, such as crystallization and tumor growth. In these fields the current simulation is still based on the high order derivative approximation. The introduction of this solver allows the simulation reflecting more complicated interactions.

Also we are interested in developing the parallel version of this solver. In practice the size of the problem is much larger than the test cases we presented in this dissertation, and it is beyond the capability of single computer. Therefore the parallelization is needed.

Another plan is to adopt this idea to finite element schemes. Due to properties of finite volume scheme we can not prove a very strong convergence result, however, in the finite element framework work, we expect to relax the requirement in the convergence proof.

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Vita

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