Numerical analysis and simulations for phase-field equations

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Numerical Analysis and Simulations for Phase-field Equations

YANG Jiang

A thesis submitted in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

Principal Supervisor: Prof. TANG Tao

Hong Kong Baptist University

July 2014
Declaration

I hereby declare that this thesis represents my own work which has been done after registration for the degree of PhD at Hong Kong Baptist University, and has not been previously included in a thesis or dissertation submitted to this or other institution for a degree, diploma or other qualifications.

Signature:  

Date: July 2014
Abstract

Research on interfacial phenomena has a long history, which has attracted tremendous interest in recent years. One of the most successful tools is the phase-field approach. As phase-field models usually involve very complex dynamics and it is nontrivial to obtain analytical solutions, numerical methods have played an important role in various simulations. This thesis is mainly devoted to developing accurate, efficient and robust numerical methods and the related numerical analysis for three representative phase-field models, namely the Allen-Cahn equation, the Cahn-Hilliard equation and the thin film models.

The first part of this thesis is mainly concentrated on the stability analysis for these three models, with particular attention to the Allen-Chan equation. We have established three stability criterion, i.e., nonlinear energy stability, $L^\infty$-stability and $L^2$-stability.

As shared by most phase-field models, one of the intrinsic properties of the Allen-Cahn and the Cahn-Hilliard equations is that they satisfy a nonlinear stability relationship, usually expressed as a time-decreasing free energy functional. We have studied several stabilized temporal discretization for both the Allen-Cahn and the Cahn-Hilliard equations so that the relevant nonlinear energy stability can be preserved. The corresponding temporal discretization schemes are linear and are of second-order accuracy. We also apply multi-step implicit-explicit methods to approximate the Allen-Cahn equation. We demonstrate that by suitably choosing the parameters in multi-step implicit-explicit methods the nonlinear energy stability can be preserved.

Apart from studying the energy stability for the Allen-Cahn equation, we also establish the numerical maximum principle for some fully discretized schemes. We further extend our analysis technique to the fractional-in-space Allen-Cahn equation. A more general Allen-Cahn-type equation with a nonlinear degenerate mobility and a logarithmic free energy is also considered.
The third stability under investigation is the $L^2$-stability. We prove that the continuum Allen-Cahn equation satisfies a uniform $L^p$-stability. Furthermore, we show that both semi-discretized Fourier Galerkin and Fourier collocation methods can inherit this stability for $p = 2$, i.e., $L^2$-stability. Based on the established $L^2$-stability, we accomplish the spectral convergence estimate for the Fourier Galerkin methods. We adopt the second-order Strang splitting schemes in the temporal direction with Fourier collocation methods to demonstrate the uniform $L^2$-stability in the fully discretized scheme.

Another contribution of this thesis is to propose a $p$-adaptive spectral deferred correction methods for the long time simulations for all three models. We develop a high-order accurate and energy stable scheme to simulate the phase-field models by combining the semi-implicit spectral deferred correction method and first-order stabilized semi-implicit schemes. It is found that the accuracy improvement may affect the overall energy stability. To compromise the accuracy and stability, a local $p$-adaptive strategy is proposed to enhance the accuracy by sacrificing some local energy stability in an acceptable level. Numerical results demonstrate the high effectiveness of our proposed numerical strategy.

**Keywords:** Phase-field models, Allen-Cahn equations, Cahn-Hilliard equations, thin film models, nonlinear energy stability, maximum principle, $L^2$-stability, adaptive simulations, stabilized semi-implicit schemes, finite difference, Fourier spectral methods, spectral deferred correction methods, convex splitting.
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Chapter 1

Introduction

1.1 Phase-field models

The phase-field model (PFM) has been proved to be extremely powerful in modeling interfacial phenomena, and it has attracted enormous attention in recent years. The key idea of PFMs is to replace the sharp interface by a thin transition layer. Specifically, PFMs take two distinct values (for instance +1 and −1) in each of the phases, with a smooth change between both values in the zone around the interface, which is then diffused with a finite width.

The origination of PFMs can date back to 1937, in which year Lev Landau first used an order parameter to describe the nature of the material at different points in space in [1, 2]. This order parameter function was the foundation for PFMs many years later. In [3], PFMs were first introduced in 1983 by George J. Fix to model first order liquid to solid phase transitions. Later, J.S. Langer compared the model to similar models in solidification theory and described the value of such a model when describing the physics of phase transitions in [4].

Besides the original applications, PFMs have been recently used to model many other physical phenomena including solid-solid transitions [12], dendritic growth [8], ferroelectric ceramics [7], dewetting and rupture of thin liquid films [14], vesicle membranes [10], planet formation [6], foams [5], infiltration of water into a porous medium [13], growth of cancerous tumors [11], phase separation of block copolymers [9], two-phase incompressible flows [89] and references therein, etc.

Solid base on mathematics and thermodynamics is one of the main reasons for
the success for PFMs. Unlike classical macroscopic models of phase transitions whose governing equations are formulated in each phase independently, PFMs describe the complex pattern evolution of the interface between two phases in the non-equilibrium state because all the governing equations are written as unified ones in the whole space of system. This elegant and clear form brings in lots of advantage in analyzing mathematically. Since transition lays in PFMs are part of the solutions, there is no extra need to track the evolving fronts. For interface-tracking models, it is not practical to track the interface directly in high dimensions.

In this thesis, we will focus on three classical and widely used PFMs, namely Allen-Cahn equations, Cahn-Hilliard equations and thin film models.

### 1.2 Allen-Cahn equations

The Allen-Cahn (AC) equation named after Allen and Cahn is a reaction-diffusion equation expressed as

$$\frac{\partial u}{\partial t} = \epsilon^2 \Delta u - f(u), \quad (x, t) \in \Omega \times (0, T], \quad (1.2.1)$$

with the initial condition

$$u|_{t=0} = u_0, \quad (1.2.2)$$

and equipped with propel boundary conditions. For simplicity, we mostly take homogeneous Dirichlet boundary conditions, periodic boundary condition or homogeneous Neumann boundary conditions in this thesis.

In problem (1.2.1)-(1.2.2), $u$ represents the concentration of one of the two metallic components of the alloy, the positive parameter $\epsilon$ represents the inter-facial width which is small compared to the characteristic length of the laboratory scale, $\Omega \subset \mathcal{R}^d \ (d = 1, 2, 3)$ is a bounded domain, and $f(u) = F'(u)$ with $F(u)$ being a given free energy, which usually has a double-well form. Two commonly used are the polynomial form

$$F(u) = \frac{1}{4}(u^2 - 1)^2 \quad (1.2.3)$$
and the logarithmic form

\[ F(u) = \frac{\theta}{2}[(1 + u) \ln(1 + u) + (1 - u) \ln(1 - u)] - \frac{\theta_c}{2} u^2, \quad (1.2.4) \]

where \( \theta < \theta_c \) are two positive constants. Scaling time with \( \epsilon \), the governing equation (1.2.1) becomes as

\[ \frac{\partial u}{\partial t} = \epsilon \Delta u - \frac{1}{\epsilon} f(u), \quad (x, t) \in \Omega \times (0, T]. \quad (1.2.5) \]

Similarly, another form can be obtained

\[ \frac{\partial u}{\partial t} = \Delta u - \frac{1}{\epsilon^2} f(u), \quad (x, t) \in \Omega \times (0, T]. \quad (1.2.6) \]

These three forms are equivalent to each other just in different scales.

The AC equation was originally introduced by Allen and Cahn in [15] to describe the motion of anti-phase boundaries in crystalline solids. The AC equation has been widely used to model various phenomena in nature. In particular, it has become a basic model equation for the diffuse interface approach developed to study phase transitions and interfacial dynamics in materials science [19, 20, 21], and it even has been applied in image inpainting [22] as well as mean curvature flows [16, 17, 18].

An important feature of the AC equation is that the problem can be characterized by the Liapunov energy functional

\[ E(u) = \int_{\Omega} \left( \frac{\epsilon}{2} |\nabla u|^2 + F(u) \right) dx \quad (1.2.7) \]

in \( L^2 \). By taking the inner product for Eq. (1.2.1) with \(-\epsilon \Delta u + f(u)\), we can obtain the energy law as

\[ \frac{\partial E(u(t))}{\partial t} = - \int_{\Omega} | - \epsilon \Delta u + f(u) |^2 dx, \quad (1.2.8) \]

which yields the following energy-decay property:

\[ E(u(t_n)) \leq E(u(t_m)), \quad \forall t_n > t_m. \quad (1.2.9) \]

Another intrinsic property of AC equations is the maximum principle. Specifically, if the initial value and boundary conditions are both bounded by constant 1, the entire solutions are also bounded by 1. Together with the nonlinear energy stability and the maximum principle, \( L^2 \)-stability will be studied in my thesis.


## 1.3 Cahn-Hilliard equations

What is now so-called Cahn-Hilliard (CH) equation was actually first formulated by van der Waals in 1983. It was totally forgotten until 1979 when it was translated by Rowlinson [23]. Over sixty years later, Cahn and Hilliard independently derived this model without knowledge of van der Waals’ work. The CH equation is given

\[
\frac{\partial u}{\partial t} = \Delta(-\epsilon^2 \Delta u + f(u)),
\]

enclosed with initial values and boundary conditions. In the most cases, two kind of double-well potential are adopted, that is, the polynomial form

\[
f(u) = u^3 - u
\]

and the logarithmic form

\[
f(u) = \frac{\theta}{2} \ln \left( \frac{1 + u}{1 - u} \right) - \theta \epsilon u.
\]

Similar as AC equations, CH equations can be viewed as an $H^{-1}$ gradient flow of the Liapunov energy functional

\[
E(u) = \int_\Omega \left( \epsilon^2 |\nabla u|^2 + F(u) \right) dx,
\]

where $F(u) = \int f(u) du$ which is the chemical free energy. The first term $\frac{\epsilon}{2} |\nabla u|^2$ is the surface free energy. Another more complicated form also draw much attention

\[
\frac{\partial u}{\partial t} = \nabla \cdot (M(u) \nabla (-\epsilon^2 \Delta u + f(u))),
\]

where $M(u)$ is a non-negative mobility. And the most common choice is the following degenerate mobility

\[
M(u) = D(1 - u^2),
\]

where $D$ is a positive constant. This non-constant mobility can describe the physics of phase separation more accurately since pure phases must have vanishing mobility.

The CH equation was originally introduced to describe the process of phase separation, by which the two components of a binary fluid spontaneously separate and
form domains pure in each component. Nowadays, it has been widely applied in
many other fields ranging from micro-film dynamics as well as bio-film structure for-
mulation, polymer flow dynamics, population dynamics, river bed formation, and
even some very large scale systems as the stellar dynamics as well as in the theory
of galaxy formation as a model for the evolution of two components of inter-galactic
material. More recently it has appeared in image processing [24, 25, 26], many com-
plicated moving interface problems in material science and fluid dynamics through a
phase-field approach [53, 27].

Due to a wide diversity of applications, many scientists, engineers and mathe-
maticians have had considerable interest in CH equations. Moreover, it was found
to be very attractive as an equation itself in mathematics thanks to the biharmonic
operator and highly nonlinear term. Under suitable initial conditions, it reproduces
two kinds of time scales dynamics, that is, a rapid spinodal decomposition process
and followed by a very long time coarsening process. Many efforts have been devoted
to the analytical studies. In [31, 32] the steady state solutions of the CH equation
were studied. The global existence of solutions to CH equations was shown by Elliott
and Sonqmu in 1986 [28]. Later, asymptotic analysis by Alikakos et al. derived the
rigorous convergence of the CH equation to the Mullins-Sekerka flow in [33]. An
interesting model named viscous CH equation derived by Novick-Cohen [34] as

\[(1 - \alpha)u_t = \Delta(f(u) - \epsilon^2 \Delta u + \alpha u_t).\]  

(1.3.7)

When \(\alpha = 1\) it becomes exactly the AC equation. But it is exact the standard CH
equation for \(\alpha = 0\).

Same as most phase-field equations, CH equations (1.3.1) satisfy a nonlinear sta-
bility relationship, expressed as

\[
\frac{dE(u(t))}{dt} = - \int_\Omega |\nabla(-\epsilon^2 \Delta u + f'(u))|^2 \, dx \leq 0.
\]  

(1.3.8)

This energy inequality is an important property for CH equations, and it is a key
stability guide to design stable numerical schemes in various simulations. Since there
is no maximum principle for the biharmonic operator, the solutions to CH equations with polynomial potential (1.3.2) is not bounded by 1 any more, which is shown in [29]. However, for the CH equation with logarithmic potential (1.3.3), solutions can totally bounded by 1 subjected with suitable initial conditions and boundary conditions.

Another important property for CH equations should be specially mentioned, that is, mass conservation, expressed as

$$\frac{d}{dt} \int_{\Omega} u \, dx = 0.$$  \hfill (1.3.9)

This differs from the AC equation, which is nonconservative for the order parameter. But conservation for the order parameter is quite important in the physics applications. Hence, the natural boundary conditions are preferred

$$\partial_n u|_{\partial \Omega} = 0, \quad \partial_n (\epsilon^2 \Delta u - f(u))|_{\partial \Omega} = 0,$$  \hfill (1.3.10)

where $n$ is the outward normal. Sometimes periodic boundary conditions are also an alterative choice.

### 1.4 Thin film models

The nonlinear diffusion thin film model (TFM) can be written as

$$\frac{\partial u}{\partial t} = -\epsilon^2 \Delta^2 u + \nabla \cdot f(\nabla u), \quad \mathbf{x} \in \Omega, \ t \in (0, T].$$  \hfill (1.4.1)

This equation also can be viewed as an $L^2$ gradient flow associated with the following energy functional

$$E(u) = \int_{\Omega} \left( \frac{1}{2} \epsilon^2 |\Delta u|^2 + F(\nabla u) \right) \, dx.$$  \hfill (1.4.2)

There are two choices in the nonlinear term, namely the polynomial form

$$F(\nabla u) = \frac{1}{4}(|\nabla u|^2 - 1)^2, \quad f(\nabla u) = -(1 - |\nabla u|^2) \nabla u,$$  \hfill (1.4.3)
and logarithmic form

\[ F(\nabla u) = -\frac{1}{2} \ln(|\nabla u|^2 + 1), \quad f(\nabla u) = -\frac{\nabla u}{1 + |\nabla u|^2}. \]  

(1.4.4)

In the equation, \( u \) represents a scaled height function of thin film in a co-moving frame and \( \epsilon \) is a positive constant. The fourth-order term models surface diffusion, and the nonlinear term represents the Ehrlich-Schwoebel effect, according to which migrating adatoms must overcome a higher energy barrier to stick to a step from an upper rather than from a lower terrace (see, e.g. \[35, 36, 37\] and references therein). This results in an uphill atom current in the dynamics and the steepening of mounds in the film. The nonlinear term (5.1.8) selects the slope of film surface. So the associated equation (1.4.1) with (5.1.8) is called the growth equation with slope selection, and correspondingly the equation (1.4.1) with (5.1.9) is called the growth equation without slope selection.

If the surface gradient \( |\nabla u| \) is small, \( \frac{1}{1+|\nabla u|^2} \approx 1 - |\nabla u|^2 \). Hence the free energy without slope selection (5.1.9) can be approximated by the one with slope selection (5.1.8). However, the interfacial dynamics governed by these two equations are different. With slope selection, (5.1.8) predicts that mound-like or pyramid structures in the surface profile tend to have a uniform, constant mound slope. On the other hand, without slope selection, (5.1.9) predicts an unbounded mound slope as \( O(t^{1/4}) \).

This model is widely applied to model epitaxial growth of thin films. See the review \[38\] for the recent history and more details about thin film growth. Apart from the similar energy stability as AC equations and CH equations below

\[ \frac{d}{dt} E(u(t)) = -||u_t||^2_2 \leq 0, \]  

(1.4.5)

there is another energy identity for the thin film model as

\[ \frac{d}{dt} ||u||^2_2 + 4E(u) + ||\nabla u||^4_4 = |\Omega|, \]  

(1.4.6)

where \( || \cdot ||_p \) is the standard \( L^p \) norm in \( \Omega \) and \( |\Omega| \) is the volume of \( \Omega \). Besides these two energy identities, mass conservation is another important property for thin film
models
\[ \frac{d}{dt} \int_{\Omega} u dx = 0, \quad (1.4.7) \]
under suitable boundary conditions, such as periodic boundary conditions.

1.5 Numerical schemes and challenges

In this section, we will briefly review some existing works in temporal schemes and numerical challenges for these three phase-field equations. This is also the motivation of this thesis. To keep the presentation terseness, we will just review several classical numerical schemes, and, for specific applications of the relevant numerical scheme, we only take the CH equation with polynomial free energy as an example. Actually, these three numerical schemes listed next are applicable for all these three models.

1.5.1 Some existing numerical schemes

I. Energy convex splitting
In [39], Eyre gives an unconditionally stable time-stepping scheme for general gradient systems. As the underlying models are gradient flows associated with the free energy, it is natural to extend Eyre’s work to these models.

For ease of notations, we denote the free energy as \( E(u) = \int_{\Omega} G(u) dx \). The key idea of energy convex splitting is to split the functional \( G(u) \) into difference of two strictly convex functions: contractive term \( G_c(u) \) and expansive term \( G_e(u) \), i.e.

\[ E(u) = E_c(u) - E_e(u) = \int_{\Omega} G_c(u) dx - \int_{\Omega} G_e(u) dx. \quad (1.5.1) \]

This decomposition must satisfies the requirement that all eigenvalues of \( J(\nabla G_e(u)) \) dominate the largest eigenvalue of \( -J(\nabla G(u)) \). Then the expansive term is handled explicitly and the contractive term implicitly. For instance, applying this technique to CH equations with polynomial free energy, we take \( G_c(u) = u^4 \) and \( G_e(u) = u^2 \),
where both two terms are convex with regard to $u$. The resulting scheme is given as

$$
\frac{u^{n+1} - u^n}{\tau} = -\epsilon^2 \Delta^2 u^{n+1} + \Delta((u^{n+1})^3 - u^n),
$$

(1.5.2)

where $\tau$ is time step. This scheme is unconditionally stable in the sense of energy and uniquely solvable.

In [40], Gomez and Hughes developed a second-order convex splitting scheme for the CH equation with logarithmic free energy. And Shen et al. proposed also a second-order convex splitting schemes for gradient flows with Ehrlich-Schwoebel type energy [41]. These two works take different technique to achieve the second-order convex splitting but both are inspired by Eyre’s work.

II. Stabilized semi-implicit schemes

To preserve the nonlinear energy stability by linear schemes, a stabilized term is usually added

$$
\frac{u^{n+1} - u^n}{\tau} = -\epsilon^2 \Delta^2 u^{n+1} + \Delta((u^n)^3 - u^n) + \beta \Delta(u^{n+1} - u^n),
$$

(1.5.3)

where $\beta$ the stabilized parameter.

In [42] Xu and Tang designed the stabilized scheme for thin film model with slope selection, in which a nonlinear relationship between the stabilized parameter and the solutions was established. Shen and Yang adopted the stabilized scheme for numerical approximation of AC and CH equations [43], where the standard energy functional was truncated by a double-well potential to guarantee the energy stability. This technique will be introduced in the following chapter.

III. Modified Crank-Nicolson schemes

The following scheme is a second-order unconditionally energy stable scheme

$$
\frac{u^{n+1} - u^n}{\tau} = -\epsilon^2 \frac{1}{2} \Delta^2 (u^{n+1} + u^n) + \Delta \left( \frac{F(u^{n+1}) - F(u^n)}{u^{n+1} - u^n} \right),
$$

(1.5.4)

where the last term can be expressed concretely as following

$$
\frac{F(u^{n+1}) - F(u^n)}{u^{n+1} - u^n} = \frac{1}{4} (u^{n+1} + u^n)[(u^{n+1})^2 + (u^n)^2] - \frac{1}{2} (u^{n+1} + u^n).
$$

(1.5.5)
The reason why we call this scheme as modified Crank-Nicolson scheme is that the term given above can be viewed as a second-order approximation to $f(u_{n+\frac{1}{2}})$. This scheme is studied in many literatures such as [30, 44, 90, 45].

Enormous efforts on numerical simulations and numerical analysis have been made for these three phase-field equations. Up to author’s knowledge, here we just list three representative temporal schemes. More details can be found in the references given above. And more numerical works will be introduced in the following chapters.

### 1.5.2 Numerical challenges

Due to small perturbed parameters $\epsilon$, high-order derivatives, nonlinearity and fruitful dynamics process involved, especially CH equations and thin film growth models, it is of great challenge in seeking accurate, efficient and robust numerical methods to simulate these phase-field models. In addition to no analytical solutions available, it is of great value for simulating these models numerically. Enormous efforts have been made to address to the following challenges in simulations of these models.

To minimize the effect of the boundary conditions and to collect enough statistical information, large computational domain is necessary. On the other hand, one has to use small space mesh grid size to capture the transition layers accurately, whose width is $o(\epsilon)$. These two together result in large systems to be solved during every time loop. Besides the constraints on mesh grid size, the fourth-order derivative will lead to a very stiff system which needs server time step size restriction to stabilize the whole simulations. If we take very small time step during the whole simulation, the efficiency problem will occur. Because the typical dynamics of these phase-field models has two stages: the first stage (rapid in time) is known as phase separation and the second (slow in time) is known as phase coarsening. Hence, adaptive temporal schemes are desired, in which large time step is necessary.

Another challenge comes from the extra requirement of nonlinear energy stability which is intrinsic to the phase field models. Numerical evidences show that violating
the energy stability may lead to wrong steady state solutions. Common numerical methods fail to satisfy this energy stability requirement, especially requiring energy-decreasing rigorously. Explicit schemes will lead to server time step size restriction. But fully implicit schemes will result in a nonlinear system which needs iterative methods to solve. Moreover, in some cases nonlinear schemes also require very small time step size to guarantee the nonlinear system uniquely solvable. Hence, linear semi-implicit schemes are preferred. However, up to author’s knowledge, linear schemes that can preserve the energy-decreasing rigorously is only first-order. Some second-order schemes need special treatment to satisfy the energy stability.
Chapter 2

Nonlinear energy stability for temporal discretizations

2.1 Introduction

In this chapter, we investigate several second-order temporal numerical schemes, particularly emphasizing on the nonlinear energy stability, for approximating the Allen-Cahn equation

$$\begin{align*}
\frac{\partial u}{\partial t} &= \Delta u - \frac{1}{\epsilon^2} f(u), \quad (x, t) \in \Omega \times (0, T], \\
\frac{\partial u}{\partial n} \bigg|_{\partial \Omega} &= 0, \\
u|_{t=0} &= u_0;
\end{align*}$$

(2.1.1)

and the Cahn-Hilliard equation

$$\begin{align*}
\frac{\partial u}{\partial t} &= \Delta(-\Delta u + \frac{1}{\epsilon^2} f(u)), \quad (x, t) \in \Omega \times (0, T], \\
\frac{\partial u}{\partial n} \bigg|_{\partial \Omega} &= 0, \quad \frac{\partial}{\partial n} \left( (\Delta u - \frac{1}{\epsilon^2} f(u)) \right) \bigg|_{\partial \Omega} = 0, \\
u|_{t=0} &= u_0.
\end{align*}$$

(2.1.2)

Numerical evidences show that violating the energy stability may lead to wrong steady state solutions. Hence, it is important to design efficient and accurate numerical schemes satisfying the energy stability. It is known that explicit schemes usually lead to very severe time step restrictions and do not satisfy a discrete energy law. One can easily design an implicit scheme that satisfies an energy law with smaller truncation errors. But it requires solving a nonlinear equation at each time step. So we shall focus our attention on the second-order implicit-explicit schemes. The advantage of
implicit-explicit schemes are that only an elliptic equation with constant coefficients needs to be solved at each time step, making it easy to implement and remarkably efficient when fast elliptic solvers are available [46, 47, 48]. In [43], Shen and Yang established the nonlinear energy stability by stabilized implicit-explicit schemes with the specially truncated double-well potential replacing the standard polynomial \( f(u) \) and provided error estimates for two fully discretized implicit schemes. In [51], Yang gave the stabilized semi-implicit scheme and the splitting scheme for the Allen-Cahn equation. For the stabilized first-order scheme, Yang provided error analysis for the Allen-Cahn equation by using the spectrum estimate. Our first objective is to design the stabilized implicit-explicit schemes that satisfy an energy law, and fully or partially relax the restriction on time steps. This work can be regarded as the extension of these papers. We focus on the linear implicit-explicit schemes for these two nonlinear equations.

On the other hand, Du and Nicolaides [44] derived a second-order accurate unconditionally stable time-stepping nonlinear scheme for the Cahn-Hilliard equation by using the finite element method. Later on, Eyre [39] derived a first-order accurate unconditionally stable time-stepping scheme and applied it to the Cahn-Hilliard equation [52]. Eyre’s method has been extensively used by the computational community and it has served as inspiration for many other time integration schemes. Other significant works, which deal with the Cahn-Hilliard equation, are due to Gomez and Hughes [40], He et al. [54], Qiao et al. [57], and so on. Other noteworthy contributions for the phase-field crystal equation or a bistable epitaxial thin film equation are due to Xu and Tang [42], Li and Liu [36], Shen and Yang [53], Qiao et al. [56, 58, 59], Hu et al. [55] respectively. It is noted that for phase field type problems Kassam and Trefethen [75] use the exponential time-differencing fourth-order Runge-Kutta method for temporal discretization, which has been demonstrated as a powerful technique.

In this chapter, we restrict our attention to potential functionals satisfying fol-
lowing conditions
\[
\max_{u \in \mathbb{R}} |f'(u)| \leq L. \tag{2.1.3}
\]
However, the commonly used quadratic Ginzburg-Landau double-well potential \( F(u) = \frac{1}{4}(u^2 - 1)^2 \) does not satisfy this conditions. One choice is to take the truncated double-well potential \( \tilde{f}(u) \) to replace it, which is expressed as follows for a given \( M \)
\[
\tilde{f}(u) = \begin{cases} 
(3M^2)u - 2M^3, & u > M, \\
(u^2 - 1)u, & u \in [-M, M], \\
(3M^2)u + 2M^3, & u < -M.
\end{cases} \tag{2.1.4}
\]
This truncated double-well potential is also adopted in [43].

The main objectives of this chapter are twofold: First, we apply the stabilized Crank-Nicolson/Adams-Bashforth scheme for approximating the Allen-Cahn equation and Cahn-Hilliard equation. For the spatial discretization, we use the standard conforming finite element method. To guarantee energy bounded, the values range of stabilized parameters are given. Moreover, optimal error estimate of the proposed second-order scheme are deduced in detail. Secondly, we investigate the first- and second-order implicit-explicit (IMEX) schemes with parameters for solving the Allen-Cahn equation. We figure out the relationship between the parameters and the nonlinear energy stability.

### 2.2 Stabilized Crank-Nicolson/Adams-Bashforth schemes

First, we introduce some notations and the standard Sobolev space. The space \( L^2(\Omega) \) is equipped with the \( L^2 \)-scalar product \( \langle \cdot, \cdot \rangle \) and \( L^2 \)-norm \( \| \cdot \|_0 \). The space \( H^1_0(\Omega) \) is endowed with the usual scalar product \( (\nabla u, \nabla v) \) and the norm \( \| \nabla u \|_0 \). We also denote by \( \| \cdot \|_r = \| \cdot \|_{0,r} \) the norm on space \( L^r(\Omega) \) with \( 1 < r < \infty \), and \( \| \cdot \|_{k,r} \) the norm on space \( W^{k,r}(\Omega) \) with \( k = 0, 1, 2, \cdots \). Given \( q \in [1, \infty) \), \( T > 0 \) and a Banach
space $W$, the space $L^q(0, T; W)$ consists of functions defined on $(0, T)$ into $W$ that are strongly $q$-integrable. The space $L^q(0, T; W)$ is equipped with the usual scalar product and norm

$$
\| \cdot \|_{L^q(0, T; W)} = \left( \int_0^T \| \cdot \|_W^q \right)^{1/q}, \quad (\cdot, \cdot) = \int_0^T (\cdot, \cdot)_W dt.
$$

Based on above definitions, for Allen-Cahn equation, its variational formulation is:

Find $u \in L^2(0, T; H^1(\Omega))$, such that

$$
\left( \frac{\partial u}{\partial t}, v \right) + \left( \nabla u, \nabla v \right) + \frac{1}{\varepsilon^2} \left( f(u), v \right) = 0, \quad \forall v \in L^2(0, T; H^1(\Omega)).
$$

(2.2.1)

We will use the conforming finite element approximation for the spatial space. Let $h > 0$ be a real positive parameter. The finite element subspace $U_h$ of $H^1(\Omega)$ is characterized by $J_h = J_h(\Omega)$, a partitioning of $\hat{\Omega}$ into triangles or quadrilaterals, assumed to be uniformly regular as $h \to 0$. Let $P_h : L^2(\Omega) \to U_h$ denote the $L^2$-orthogonal projection such that

$$
(P_h v, v_h) = (v, v_h), \quad v \in L^2(\Omega), \ v_h \in U_h,
$$

and let us define a projection operator $I_h : H^1(\Omega) \to U_h$ by

$$
(\nabla (v - I_h v), \nabla \varphi) = 0, \quad (\nabla (v - I_h v), 1) = 0, \quad \forall \varphi \in U_h.
$$

It is well known that the following estimates hold:

$$
\| v - P_h \|_0 \leq ch^m \| v \|_m, \quad \forall v \in H^m(\Omega), \ m \geq 0,
$$

$$
\| v - I_h \|_i \leq ch^{m-i} \| v \|_m, \ i = 0, 1, \quad \forall v \in H^m(\Omega), \ m \geq 1.
$$

### 2.2.1 Stabilized schemes for the Allen-Cahn equation

Note that Shen and Yang used a stabilized second-order backward difference formula (BDF) with adding the second-order term $\frac{\delta}{\varepsilon^2} (u^{n+1} - 2u^n + u^{n-1})$

$$
\frac{1}{2\delta t} \left( 3u^{n+1} - 4u^n + u^{n-1}, v \right) + \left( \nabla u^{n+1}, \nabla v \right) + \frac{\delta}{\varepsilon^2} (u^{n+1} - 2u^n + u^{n-1})
$$

$$
+ \frac{1}{\varepsilon^2} \left( 2f(u^n) - f(u^{n-1}), v \right) = 0, \quad \forall v \in H^1(\Omega),
$$

(2.2.2)
And under the condition $\delta t \leq \frac{2^2}{3L}$, the following stable energy law of this stabilized scheme holds

$$E(u^{n+1}) - E(u^n) + \left(\frac{1}{4\delta t} + \frac{S + L}{2\epsilon^2}\right)(||u^{n+1} - u^n||^2 - ||u^n - u^{n-1}||^2) \leq 0, \forall n \geq 1. \quad (2.2.3)$$

Inspired by the above scheme, we consider the following stabilized Crank-Nicolson/Adam-Bashforth (C-N/A-B) schemes:

**Algorithm I (Stabilized second-order C-N/A-B schemes)**

$$\frac{1}{\delta t}(u^{n+1} - u^n, v) + \frac{S}{\epsilon^2}(u^{n+1} - 2u^n + u^{n-1})$$

$$+ \frac{1}{\epsilon^2}f(u^n) - \frac{1}{\epsilon}f(u^{n-1}), v = 0, \forall v \in H^1(\Omega), \quad (2.2.4)$$

**Lemma 2.1.** Under the condition

$$\delta t \leq \frac{\epsilon^2}{L}, \quad (2.2.5)$$

then the following stable energy law of Algorithm I holds:

$$\tilde{E}(u^{n+1}) \leq \tilde{E}(u^n), \quad (2.2.6)$$

where the modified energy $\tilde{E}(u^n)$ is defined as

$$\tilde{E}(u^n) = E(u^n) + \frac{L + 2S}{4\epsilon^2} ||u^n - u^{n-1}||^2, \forall n \geq 1 \quad (2.2.7)$$

**Proof.** Taking $v = u^{n+1} - u^n$ and using the Taylor expansion, we have

$$E(u^{n+1}) - E(u^n) + \left(\frac{1}{\delta t} + \frac{S}{2\epsilon^2}\right)||u^{n+1} - u^n||_0^2 + \frac{S}{2\epsilon^2}(||u^{n+1} - 2u^n + u^{n-1}||_0^2 - ||u^n - u^{n-1}||_0^2)$$

$$= \frac{1}{\epsilon^2}( \int_{u^n}^{u^{n+1}} f'(s)(u^{n+1} - s)ds, 1) - \frac{1}{2\epsilon^2}( \int_{u^n}^{u^{n+1}} f'(s)ds, u^{n+1} - u^n)$$

$$\leq \frac{L}{2\epsilon^2}( ||u^n - u^{n+1}||_0^2 + ||u^{n+1} - u^n||_0 ||u^n - u^{n-1}||_0)$$

$$\leq \frac{L}{2\epsilon^2}( ||u^n - u^{n+1}||_0^2 + \frac{1}{2} ||u^n - u^{n-1}||_0^2).$$

which implies the desired results.

Next, we use finite element approximation for the spacial variables, and establish error estimates for the fully discrete versions of Algorithm I. Subsequently, $C$ (with or without a subscript) will denote a positive constant, which may stand for different values at its different occurrences.
Theorem 2.1. Assume that $u \in C(0,T; H^m(\Omega))$, $u_t \in L^2(0,T; H^m(\Omega)) \cap L^2(0,T; L^2(\Omega))$, $u_{tt} \in L^2(0,T; H^1(\Omega))$ and $u_{ttt} \in L^2(0,T; H^{-1}(\Omega))$. Then the following error estimate holds

$$
\|u^n - u_h^n\|_0 + \delta t \| \nabla (u^{n+\frac{1}{2}} - u_h^{n+\frac{1}{2}}) \|_0 \leq C(\delta t^2 + h^2),
$$

where $C$ is a positive constant depend on $\varepsilon$, $T$, $u$ and its derivatives.

Proof. Setting $u^n(\cdot) = u(\cdot, t_n)$. Let us denote

$$
\hat{e}^n = u^n - I_h u^n, \quad e^n = I_h u^n - u_h^n,
$$

$$
\bar{e} = u^n - u_h^n = \hat{e}^n + e^n, \quad e^{n+\frac{1}{2}} = \frac{1}{2}(e^n + e^{n+1}).
$$

Now, we introduce the fully discrete scheme:

Find $u_h \in U_h \subset H^1(\Omega)$, such that

$$
\frac{1}{\delta t}(u_h^{n+1} - u_h^n, v_h) + \frac{1}{2}(\nabla (u_h^{n+1} + u_h^n), \nabla v_h) + \frac{\delta^2}{2}(u_h^{n+1} - 2u_h^n + u_h^{n-1}, v_h)
+ \frac{1}{\varepsilon^2}(f(u_h^n) - \frac{1}{2}f(u_h^{n-1}), v_h) = 0, \quad \forall v_h \in V_h \subset H^1(\Omega),
$$

(2.2.8)

Define the truncation error

$$
\frac{u(t_{n+1}) - u(t_n)}{\delta t} - u_t(t_{n+\frac{1}{2}}) = R_1^{n+\frac{1}{2}},
$$

(2.2.9)

$$
\Delta u(t_{n+\frac{1}{2}}) - \Delta(\frac{u(t_{n+1}) + u(t_n)}{2}) = R_2^{n+\frac{1}{2}}.
$$

(2.2.10)

By using the Taylor expansion with integral residual, it is easy to show that

$$
\|R^{n+\frac{1}{2}}_s\|_s^2 \leq \delta t^3 \int_{t_n}^{t_{n+1}} \|u_{ttt}(t)\|_s^2 dt, \quad s = -1, 0,
$$

(2.2.11)

$$
\|R^{n+\frac{1}{2}}_s\|_s^2 \leq \delta t^3 \int_{t_n}^{t_{n+1}} \|u_t(t)\|_{s+2}^2 dt, \quad s = -1, 0.
$$

(2.2.12)

Subtracting Eq. (2.2.4) from Eq. (2.2.8) at $t^{n+\frac{1}{2}}$, we have

$$
\begin{align*}
&\frac{1}{\delta t}(e^{n+1} - e^n, v_h) + (\nabla e^{n+\frac{1}{2}}, \nabla v_h) + \frac{\delta^2}{2}(e^{n+1} - 2e^n + e^{n-1}, v_h) \\
&= (R^{n+\frac{1}{2}}_1 + R^{n+\frac{1}{2}}_2, v_h) + \frac{1}{\delta t}((I - I_h)(u^{n+1} - u^n), v_h) \\
&+ \frac{\delta}{\varepsilon^2}(u^{n+1} - 2u^n + u^{n-1}, v_h) - \frac{\delta^2}{2}(I - I_h)(u^{n+1} - 2u^n + u^{n-1}, v_h) \\
&+ \frac{1}{\varepsilon^2}(f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u_h^n) + \frac{1}{2}f(u_h^{n-1}), v_h)
\end{align*}
$$

(2.2.13)
Taking \( v_h = 2\delta te^{n+\frac{1}{2}} \) in Eq. (2.2.13), we have
\[
(1 + \frac{8\delta}{2\epsilon})(\|e^{n+1}\|_0^2 - \|e^n\|_0^2) + 2\delta t\|\nabla e^{n+\frac{1}{2}}\|_0^2 = 2\delta t(R_1^{n+\frac{1}{2}} + R_2^{n+\frac{1}{2}}, e^{n+\frac{1}{2}}) \\
+2((I - I_h)(u^{n+1} - u^n), e^{n+\frac{1}{2}}) + \frac{2\delta S}{\epsilon^2}(u^{n+1} - 2u^n + u^{n-1}, e^{n+\frac{1}{2}}) \\
-\frac{2\delta S}{\epsilon^2}(I - I_h)(u^{n+1} - 2u^n + u^{n-1}), e^{n+\frac{1}{2}}) + \frac{2\delta S}{\epsilon^2}(e^n - e^{n-1}, e^{n+\frac{1}{2}}) \\
+\frac{2\delta}{\epsilon^2}(f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u^n) + \frac{1}{2}f(u^{n-1}), e^{n+\frac{1}{2}}) = \sum_{i=1}^6 I_i.
\]

Using the Cauchy-Schwarz inequality and Young inequality, we can estimate the right terms \( I_i \) respectively as follows
\[
I_1 \leq 2\delta t\|R_1^{n+\frac{1}{2}} + R_2^{n+\frac{1}{2}}\|_{-1}\|e^{n+\frac{1}{2}}\|_1 \\
\leq \delta t\|\nabla e^{n+\frac{1}{2}}\|_0^2 + C\delta t(\|R_1^{n+\frac{1}{2}}\|_2^2 + \|R_2^{n+\frac{1}{2}}\|_2^2).
\]
\[
I_2 \leq 2\|(I - I_h)(u^{n+1} - u^n)\|_0\|e^{n+\frac{1}{2}}\|_0 \\
\leq \frac{\delta}{\epsilon^2}\|e^{n+\frac{1}{2}}\|_0^2 + C\epsilon^2 \int_{t_n-1}^{t_{n+1}} \|(I - I_h)u_t(s)\|_0^2 ds,
\]
\[
I_3 \leq \frac{2\delta S}{\epsilon^2}\|u^{n+1} - 2u^n + u^{n-1}\|_0\|e^{n+\frac{1}{2}}\|_0 \\
\leq \frac{\delta}{\epsilon^2}\|e^{n+\frac{1}{2}}\|_0^2 + \frac{CS^2\delta t}{\epsilon^2} \int_{t_n-1}^{t_{n+1}} \|u_t(s)\|_0^2 ds
\]
\[
I_4 \leq \frac{2\delta S}{\epsilon^2}\|(I - I_h)(u^{n+1} - 2u^n + u^{n-1})\|_0\|e^{n+\frac{1}{2}}\|_0 \\
\leq \frac{\delta}{\epsilon^2}\|e^{n+\frac{1}{2}}\|_0^2 + \frac{CS^2\delta t}{\epsilon^2} \int_{t_n-1}^{t_{n+1}} \|(I - I_h)u_t(s)\|_0^2 ds,
\]
\[
I_5 \leq \frac{2\delta S}{\epsilon^2}\|e^n - e^{n-1}\|_0\|e^{n+\frac{1}{2}}\|_0 \\
\leq \frac{\delta}{\epsilon^2}\|e^{n+\frac{1}{2}}\|_0^2 + \frac{CS^2\delta t}{\epsilon^2}\|e^n - e^{n-1}\|_0^2
\]
\[
I_6 \leq \frac{2\delta S}{\epsilon^2}\|f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u^n) + \frac{1}{2}f(u^{n-1})\|_0\|e^{n+\frac{1}{2}}\|_0 \\
\leq \frac{\delta}{\epsilon^2}\|e^{n+\frac{1}{2}}\|_0^2 + \frac{\delta}{\epsilon^2}\|f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u^n) + \frac{1}{2}f(u^{n-1})\|_0^2 \\
= \frac{\delta}{\epsilon^2}\|e^{n+\frac{1}{2}}\|_0^2 + \frac{\delta}{\epsilon^2}I_7,
\]
where
\[
I_7 \leq \|f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u^n) + \frac{1}{2}f(u^{n-1})\|_0^2 + \|\frac{3}{2}f(u^n) - \frac{3}{2}f(u^{n-1})\|_0^2 + \frac{1}{2}f(u^{n-1})\|_0^2 \\
\leq \|f(u^{n+\frac{1}{2}}) - \frac{1}{2}f(u^{n+1}) + f(u^n)\|_0^2 + \|\frac{1}{2}f(u^{n+1}) + f(u^n) - \frac{1}{2}f(u^{n-1}) + \frac{1}{2}f(u^{n-1})\|_0^2 \\
+ CL^2(\|u^n - u^n\|_0^2 + \|u^{n-1} - u^{n-1}\|_0^2) \\
\leq CL\delta^2 \int_{t_n-1}^{t_{n+1}} \|u_t(s)\|_0^2 ds + CL^2(\|e^n\|_0^2 + \|\tilde{e}^n\|_0^2 + \|e^{n-1}\|_0^2 + \|\tilde{e}^{n-1}\|_0^2).
Combining these into Eq. (2.2.14), we obtain

\[
(1 + \frac{S_{\delta t}}{2\varepsilon}) \left( \|e^{n+1}\|_0^2 - \|e^n\|_0^2 \right) + \delta t \|\nabla e^{n+\frac{1}{2}}\|_0^2 \\
\leq C\delta t \left( \|R_1^{n+\frac{1}{2}}\|_{L^2}^2 + \|R_2^{n+\frac{1}{2}}\|_{L^2}^2 \right) + Ce^2 \int_{t_n}^{t_{n+1}} \|(I - \Pi_h)u_t(s)\|_0^2 ds \\
+ \frac{C\delta t^4}{\varepsilon} \int_{t_{n-1}}^{t_n} \|u_t(s)\|_2^2 ds + \frac{CS^2\delta t^4}{\varepsilon} \int_{t_{n-1}}^{t_n} \|(I - I_h)u_t(s)\|_0^2 ds \\
+ \frac{C\delta t}{\varepsilon} \left( \|e^n\|_0^2 + \|\hat{e}^n\|_0^2 + \|e^{n-1}\|_0^2 + \|\hat{e}^{n-1}\|_0^2 \right).
\]

(2.2.15)

Summing up the above inequality for \( n = 1, \ldots, N - 1 \), and using the interpolation error estimate, we obtain

\[
(1 + \frac{S_{\delta t}}{2\varepsilon}) \left( \|e^N\|_0^2 - \|e^1\|_0^2 \right) + \delta t \sum_{n=1}^{N-1} \|\nabla e^{n+\frac{1}{2}}\|_0^2 \\
\leq C\delta t^4 \left( \|u_{tt}\|_{L^2(0,T;H^{-1})} + \|u_t\|_{L^2(0,T;H^1)} \right) + Ce^2 \delta t \left( \|u_t\|_{L^2(0,T;L^2)} \right) \\
+ \frac{C\delta t^4}{\varepsilon} \left( \|u_t\|_{L^2(0,T;L^2)} + \|u_t\|_{L^2(0,T;L^2)} \right) + \frac{C\delta t}{\varepsilon} \sum_{n=0}^{N-1} \left( \|e^n\|_0^2 + \|\hat{e}^n\|_0^2 + \|e^{n-1}\|_0^2 + \|\hat{e}^{n-1}\|_0^2 \right).
\]

(2.2.16)

If we apply the discrete Gronwall lemma to the above inequality and use the triangular inequality, we can get the desired result. \( \square \)

### 2.2.2 Stabilized schemes for the Cahn-Hilliard equation

For Cahn-Hilliard equations, its mixed variational formulation is: Find \( u, w \in L^2(0, T; H^1(\Omega)) \) such that

\[
\begin{align*}
(\frac{\partial u}{\partial t}, v) + (\nabla w, \nabla v) &= 0, \quad \forall v \in L^2(0, T; H^1(\Omega)), \\
(\nabla u, \nabla \phi) + \frac{1}{\varepsilon} (f(u), \phi) &= (w, \phi), \quad \forall \phi \in L^2(0, T; H^1(\Omega)).
\end{align*}
\]

(2.2.17)

**Algorithm II** (Stabilized second-order C-N/A-B schemes)

Find \((u^{n+1}, w^{n+1}) \in H^1(\Omega) \times H^1(\Omega)\), such that

\[
\begin{align*}
\frac{1}{\varepsilon} (w^{n+1} - w^n, v) + (\nabla w^{n+1}, \nabla v) &= 0, \\
(\nabla u^{n+\frac{1}{2}}, \nabla \phi) + \frac{S}{\varepsilon} (u^{n+1} - 2u^n + u^{n-1}, \phi) + \frac{1}{\varepsilon^2} (\frac{3}{2} f(u^n) - \frac{1}{2} f(u^{n-1}), \phi) &= (w^{n+1}, \phi).
\end{align*}
\]

(2.2.18)

for all \((v, \phi) \in H^1(\Omega) \times H^1(\Omega)\), where \( u^{n+\frac{1}{2}} = \frac{1}{2} (u^{n+1} + u^n) \).
Next, we use finite element approximation for the spacial variables, and establish error estimates for the fully discrete versions of Algorithm II.

Find \((u_h^{n+1}, w_h^{n+1}) \in U_h \times U_h\), such that for all \((v_h, \phi_h) \in V_h \times V_h\),

\[
\begin{align*}
\frac{1}{\delta t}(u_h^{n+1} - u_h^n, v_h) + (\nabla w_h^{n+1}, \nabla v_h) &= 0, \\
(\nabla u_h^{n+\frac{1}{2}}, \nabla \phi_h) + \frac{S}{\varepsilon^2}(u_h^{n+1} - 2u_h^n + u_h^{n-1}, \phi_h) + \frac{1}{\varepsilon^2}(\frac{3}{2}f(u_h^n) - \frac{1}{2}f(u_h^{n-1}), \phi_h) &= (w_h^{n+1}, \phi_h)
\end{align*}
\]

We denote

\[
\begin{align*}
\bar{e}^n &= u(t_n) - u_h(t_n), & e^n &= u_h(t_n) - u^n, \\
\bar{\eta}^n &= w(t_n) - w_h(t_n), & \eta^n &= w_h(t_n) - w^n, \\
\bar{\eta}^{n+\frac{1}{2}} &= w(t_{n+\frac{1}{2}}) - w_h(t_{n+\frac{1}{2}}), & \eta^{n+\frac{1}{2}} &= w_h(t_{n+\frac{1}{2}}) - w_h^{n+1},
\end{align*}
\]

**Theorem 2.2.** Assume that \(u, w \in C(0, T; H^1(\Omega))\), \(u_t \in L^2(0, T; H^1(\Omega)) \cap L^2(0, T; L^2(\Omega))\), \(u_{tt} \in L^2(0, T; H^1(\Omega))\) and \(u_{ttt} \in L^2(0, T; H^{-1}(\Omega))\). Then the following error estimate holds

\[
\|u^n - u_h^n\|_0 + \delta t\|\nabla (w^{n+\frac{1}{2}} - w_h^{n+\frac{1}{2}})\|_0 \leq C(\delta t^2 + h^2),
\]

where \(C\) is a positive constant depend on \(\varepsilon, T, u\) and its derivatives.

**Proof.** Subtracting (2.2.18) from (2.2.19) at \(t^{n+\frac{1}{2}}\), we find

\[
\begin{align*}
(e^{n+1} - e^n, v_h) + (\nabla \eta^{n+\frac{1}{2}}, \nabla v_h) &= (R_1^{n+\frac{1}{2}}, v_h) - (\nabla \bar{\eta}^{n+\frac{1}{2}}, \nabla v_h) - (\frac{e^{n+1} - e^n}{\delta t}, v_h), \\
(\nabla e^{n+\frac{1}{2}}, \nabla \phi_h) + \frac{S}{\varepsilon^2}(f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u_h^n) + \frac{1}{2}f(u_h^{n-1}), \phi_h) \\
&+ \frac{S}{\varepsilon^2}(e^{n+1} - 2e^n + e^{n-1}, \phi_h) \\
&= (R_2^{n+\frac{1}{2}}, \phi_h) + (\eta^{n+\frac{1}{2}} + \bar{\eta}^{n+\frac{1}{2}}, \phi_h) - (\nabla e^{n+\frac{1}{2}}, \nabla \phi_h) \\
&+ \frac{S}{\varepsilon^2}(u^{n+1} - 2u^n + u^{n-1}, \phi_h) \\
&- \frac{S}{\varepsilon^2}((I - I_h)(u^{n+1} - 2u^n + u^{n-1}), \phi_h).
\end{align*}
\]

Taking \(v_h = 2\delta t e^{n+\frac{1}{2}}\) and \(\phi_h = -2\delta t \eta^{n+\frac{1}{2}}\) and summing up the two identities, we
have

\[ \frac{\|e^{n+1}\|^2_0}{2} - \|e^n\|^2_0 + 2\delta t\|\eta^{n+\frac{1}{2}}\|^2_0 = 2\delta t(R_1^{n+\frac{1}{2}}, e^{n+\frac{1}{2}}) - 2(e^{n+1} - e^n, e^{n+\frac{1}{2}}) + 2\delta t \frac{S}{\epsilon}(e^{n+1} - e^n + e^{n-1}, \eta^{n+\frac{1}{2}}) + 2\delta t \frac{1}{\epsilon}(f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u^n) + \frac{1}{2}f(u^{n-1}), \eta^{n+\frac{1}{2}}) - 2\delta t(R_2^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}}) \]

(2.2.21)

\[ -2\delta t(\eta^{n+\frac{1}{2}}, \eta^{n+\frac{1}{2}}) - 2\delta t \frac{S}{\epsilon}(u^{n+1} - 2u^n + u^{n-1}, \eta^{n+\frac{1}{2}}) + \delta t \frac{S}{\epsilon}(\eta^{n+\frac{1}{2}} - (I - \eta)(u^{n+1} - 2u^n + u^{n-1}), \eta^{n+\frac{1}{2}}) =: \sum_{i=1}^{8} \Pi_i \]

Next we estimate the right terms:

\[ \Pi_1 \leq C\delta t\|e^{n+\frac{1}{2}}\|^2_0 + C\delta t^4 \int_{t_n}^{t_{n+1}} \|u_{tt}(s)\|^2_0 ds; \]
\[ \Pi_2 \leq C\|e^{n+\frac{1}{2}}\|_0 \|(I - \eta)(u^{n+1} - u^n)\|_0 \]
\[ \leq C\delta t\|e^{n+\frac{1}{2}}\|^2_0 + C \int_{t_n}^{t_{n+1}} \|(I - \eta)u_t(s)\|^2_0 ds; \]
\[ \Pi_3 \leq 2\delta t \frac{S}{\epsilon^2}\|e^{n+1} - 2e^n + e^{n-1}\|_0 \|\eta^{n+\frac{1}{2}}\|_0 \]
\[ \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|_0 + \frac{C\delta t^4}{\epsilon^2}\|e^{n+1} - 2e^n + e^{n-1}\|_0^2; \]
\[ \Pi_4 \leq 2\delta t \frac{1}{\epsilon^2}\|f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u^n) + \frac{1}{2}f(u^{n-1})\|_0 \|\eta^{n+\frac{1}{2}}\|_0 \]
\[ \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|_0 + \frac{C\delta t^4}{\epsilon^2}\|f(u^{n+\frac{1}{2}}) - \frac{3}{2}f(u^n) + \frac{1}{2}f(u^{n-1})\|_0 \]
\[ \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|_0 + \frac{C\delta t^4}{\epsilon^2}\int_{t_{n-1}}^{t_{n+1}} \|u_{tt}(s)\|^2_0 ds \]
\[ + CL^2(\|e^n\|_0^2 + \|\bar{e}_n\|_0^2 + \|e^{n-1}\|_0^2 + \|\bar{e}^{n-1}\|_0^2); \]
\[ \Pi_5 \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|^2_0 + C\delta t^4 \int_{t_n}^{t_{n+1}} \|u_{tt}(s)\|^2_0 ds; \]
\[ \Pi_6 \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|^2_0 + C\delta t\|\bar{u}^{n+\frac{1}{2}}\|_0^2; \]
\[ \Pi_7 \leq 2\delta t \frac{S}{\epsilon^2}\|u^{n+1} - 2u^n + u^{n-1}\|_0 \|\eta^{n+\frac{1}{2}}\|_0 \]
\[ \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|^2_0 + \frac{C\delta t^4}{\epsilon^2}\|u^{n+1} - 2u^n + u^{n-1}\|_0^2 \]
\[ \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|^2_0 + \frac{C\delta t^4}{\epsilon^2}\int_{t_{n-1}}^{t_{n+1}} \|u_{tt}(s)\|^2_0 ds; \]
\[ \Pi_8 \leq \delta t \frac{S}{\epsilon^2}(I - \eta)(u^{n+1} - 2u^n + u^{n-1})\|\eta^{n+\frac{1}{2}}\|_0 \]
\[ \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|^2_0 + \frac{C\delta t^4}{\epsilon^2}\|(I - \eta)(u^{n+1} - 2u^n + u^{n-1})\|_0^2 \]
\[ \leq \frac{\delta t^4}{\epsilon^2}\|\eta^{n+\frac{1}{2}}\|^2_0 + \frac{C\delta t^4}{\epsilon^2}\int_{t_{n-1}}^{t_{n+1}} \|(I - \eta)u_{tt}(s)\|^2_0 ds. \]
Combing the above inequalities into Eq. (2.2.21), we have

$$\left\| \mathbf{e}^{n+1} \right\|_0^2 - \left\| \mathbf{e}^n \right\|_0^2 + \delta t \left\| \eta^{n+\frac{1}{2}} \right\|_0^2 \leq C \delta t \left\| \mathbf{e}^{n+\frac{1}{2}} \right\|_0^2 + C \delta t^4 \int_{t_n}^{t_{n+1}} \left\| u_{ttt}(s) \right\|_0^2 ds$$

$$+ C \int_{t_n}^{t_{n+1}} \|(I - I_h)u_t(s)\|_0^2 ds + \frac{C \delta t^2}{\epsilon^4} \left\| \mathbf{e}^{n+1} - 2\mathbf{e}^n + \mathbf{e}^{n-1} \right\|_0^2$$

$$+ \frac{C \delta t^4}{\epsilon^2} \int_{t_{n-1}}^{t_{n+1}} \left\| u_{tt}(s) \right\|_0^2 ds + \frac{C \delta t^4}{\epsilon^2} \int_{t_{n-1}}^{t_{n+1}} \left\| (I - I_h)u_{tt}(s) \right\|_0^2 ds$$

$$+ CL^2 \left( \left\| \mathbf{e}^n \right\|_0^2 + \left\| \hat{\mathbf{e}}^n \right\|_0^2 + \left\| \mathbf{e}^{n-1} \right\|_0^2 + \left\| \hat{\mathbf{e}}^{n-1} \right\|_0^2 \right) . \tag{2.22}$$

We can then conclude by applying the discrete Gronwall lemma to the above inequality, and by using the triangular inequality and interpolation approximation. Now we end the proof of theorem.

\[ \square \]

### 2.2.3 Numerical tests for convergence rate

In this section, we present some numerical results for two-dimensional cases to illustrate the theoretical results obtained in the previous section.

**Example 2.1. 2D Allen-Cahn equation** The initial condition is taken as the trigonometric function with very small amplitude,

$$u_0(x, y) = 0.05 \sin x \sin y,$$

and the problem is subject to periodic boundary condition. The parameter $\epsilon$ is 0.1. $\Omega = [0, 2\pi] \times [0, 2\pi]$.

This example is designed to study the accuracy and the efficiency of C-N/A-B scheme. First, we test the numerical accuracy in time and space respectively. Since the exact solution is unknown, we take the numerical result obtained on $P_1$-conforming element and the spatial step $h = 2\pi/128$ and time step $\delta t = 1.0 e^{-3}$ as the basic solution. Taking $S = 0$ and $S = 1$ respectively, Table 2.1 and Table 2.2 show the $L^2$-errors obtained using different constant time steps at $T = 0.01$. It is seen that the numerical scheme gives optimal error in $L^2$-norm for this two-dimensional Allen-Cahn problem. Moreover, we show the $L^2$-errors obtained using $\delta t = 1.0 e^{-4}$ and different constant spatial steps at $T = 0.01$ in Table 2.3 and Table 2.4. We also
Table 2.1: Numerical results of time discretization for 2D Allen-Cahn equation as $S=0$.

Table 2.2: Numerical results of time discretization for 2D Allen-Cahn equation as $S=1$.

obtain the optimal error estimate for different $S$. Furthermore, we find the spatial error are similar for different $S$ if the time step is small enough. The key reason is that the time error cancel out each other.

Figure 2.1 shows the trend of energy evolution for $S = 0$ and $S = 1$ respectively. In Fig. 2.1(a), when $\delta t = 0.01$, the energy is oscillating but not decreasing. When $\delta t = 0.005$, the energy is decreasing, and when $\delta t = 0.001$, the energy is decreasing. However, in 2.1(b), the energy-decreasing property is preserved quite well.

Example 2.2. 2D Cahn-Hilliard equation The initial condition is taken as the
\[ h = \frac{2\pi}{8} \]
\[ h = \frac{2\pi}{16} \]
\[ h = \frac{2\pi}{32} \]
\[ h = \frac{2\pi}{64} \]
\[ h = \frac{2\pi}{128} \]

\[ \| u_{h,\delta t} - u_{h/2,\delta t} \| \]
\[ 4.208e-2 \]
\[ 1.094e-2 \]
\[ 2.760e-3 \]
\[ 6.918e-4 \]
\[ 1.730e-4 \]

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Table 2.4: Numerical results of spatial discretization for 2D Allen-Cahn equation as $S=1$.

Figure 2.1: (a). The trend of energy evolution of 2D Allen-Cahn equation for $S = 0$. (b). The trend of energy evolution of 2D Allen-Cahn equation for $S = 1$. 
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<th>$\delta t/4$</th>
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<td>1.99</td>
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</table>

Table 2.5: Numerical results of time discretization for 2D Cahn-Hilliard equation as $S = 0$.

Trigonometric function with very small amplitude,

$$u_0(x, y) = 0.1(\sin(3x) \sin(2y) + \sin(5x) \sin(5y)),$$

and the problem is subject to periodic boundary condition. The parameter $\epsilon$ is 0.1. $\Omega = [0, 2\pi] \times [0, 2\pi]$.

This example is designed to study the accuracy and the efficiency of C-N/A-B scheme. First, we test the numerical accuracy in time and space. We take the numerical result obtained on $P_1$-conforming element and the spatial step $h = 2\pi/128$. Taking $S = 0$ and $S = 1$, Table 2.5 and Table 2.6 show the $L^2$-errors obtained using $\delta t = 1.0e-6$ and different constant time steps at $T = 1.0e-4$. It is seen that the numerical scheme gives optimal error in $L^2$-norm for this two-dimensional Cahn-Hilliard problem.

### 2.3 Multi-step implicit-explicit Methods for the Allen-Cahn equation

It is observed that the Allen-Cahn equation involves a small positive parameter in the diffusion term, which normally leads to a stiff system after spatial discretizations. In this case, the implicit-explicit (IMEX) technique, which has been introduced for
Table 2.6: Numerical results of time discretization for 2D Cahn-Hilliard equation as $S = 1$.

time dependent partial differential equations, usually can play an important role, see, e.g., [46, 47]. The IMEX schemes use an implicit scheme for the diffusion term and an explicit scheme for the convection term. Some schemes of this type were proposed and analyzed as far back as the late 1970’s, and we refer to [48, 49, 50] for recent developments. In this section, we will consider applying explicit-implicit schemes to approximate the Allen-Cahn equation. Our goal is to obtain stable first- and second-order time-accurate schemes.

### 2.3.1 General linear multi-step implicit-explicit schemes

Assume that all the spatial derivatives in the Allen-Cahn equation (1.2.1) have been discretized by certain difference methods. This gives rise to a large system of ordinary differential equations in time which typically has the form

$$
\frac{dU}{dt} = \epsilon AU + B(U),
$$

(2.3.1)

where $A$ is a constant matrix and $B$ is a nonlinear operator for $U$. We now introduce $k$-step implicit-explicit schemes for Eq. (2.3.1). Letting $\tau$ be the time-step and $U^n$ denote the approximate solution at $t_n = n\tau$, we may obtain from (2.3.1) that

$$
\frac{1}{\tau} \left( U^{n+1} + \sum_{j=0}^{k-1} \alpha_j U^{n-j} \right) = \epsilon \sum_{j=-1}^{k-1} \beta_j U^{n-j} + \sum_{j=0}^{k-1} \gamma_j B(U^{n-j}),
$$

(2.3.2)
where $\beta_{-1} \neq 0$. Assume that function $U(t)$ is smooth enough. Using Taylor expansion at $t_n = n\tau$ gives the following truncation error

$$
\frac{1}{\tau} \left( 1 + \sum_{j=0}^{k-1} \alpha_j \right) U(t_n) + \left( 1 - \sum_{j=1}^{k-1} j\alpha_j \right) U^{(1)}(t_n) + \cdots + \frac{\tau^{p-1}}{p!} \left( 1 + \sum_{j=1}^{k-1} (-j)^p \alpha_j \right) U^{(p)}(t_n)
$$

$$
- \epsilon \sum_{j=1}^{k-1} \beta_j A U(t_n) - \tau \epsilon \left( \beta_{-1} - \sum_{j=1}^{k-1} \beta_j \right) A \dot{U}(t_n) - \cdots
$$

$$
- \frac{\tau^{p-1}}{(p-1)!} \epsilon \left( \beta_{-1} + \sum_{j=0}^{k-1} \beta_j (-j)^{p-1} \right) A U^{(p-1)}(t_n) - \sum_{j=0}^{k-1} \gamma_j B(U(t_n))
$$

$$
+ \tau \sum_{j=1}^{k-1} j\gamma_j B^{(1)} - \cdots - \frac{\tau^{p-1}}{(p-1)!} \sum_{j=1}^{k-1} (-j)^p \gamma_j B^{(p-1)} = o(\tau^p),
$$

(2.3.3)

where $U^{(i)}(t_n)$ denotes the $i$th-order derivative of function $U$ at $t_n$, and $B^{(i)}$ denotes the $i$th-order derivative of function $B$ at $u(t_n)$, $i \geq 1$. Applying the original equation to the truncation error, we obtain $p$th-order scheme provided the following conditions hold:

$$
1 + \sum_{j=0}^{k-1} \alpha_j = 0,
$$

$$
1 - \sum_{j=1}^{k-1} j\alpha_j = \sum_{j=1}^{k-1} \beta_j = \sum_{j=0}^{k-1} \gamma_j,
$$

$$
\vdots
$$

$$
\frac{1}{p!} \left( 1 + \sum_{j=1}^{k-1} (-j)^p \alpha_j \right) = \frac{1}{(p-1)!} \left( \beta_{-1} + \sum_{j=1}^{k-1} \beta_j (-j)^{p-1} \right) = \frac{1}{(p-1)!} \sum_{j=1}^{k-1} (-j)^{p-1}.
$$

(2.3.4)

It follows from [46, 47] that the family of $k$-step implicit-explicit schemes of order $k$ has $k$ parameters, and the $k$-step implicit-explicit scheme can not have order of accuracy greater than $k$. Below we will present the first- and second-order implicit-explicit schemes with parameters by solving the underdetermined system (2.3.4).

The first-order implicit-explicit schemes for ODEs can be written as

$$
\frac{U^{n+1} - U^n}{\tau} = \epsilon A[\alpha U^{n+1} + (1 - \alpha)U^n] + B(U^n)
$$

(2.3.5)

where $\alpha$ is a free parameter. Here we restrict $\alpha > 0$ to prevent large truncation error and ensure the schemes having good stability.
We point out that choosing $\alpha = 1$ the backward Euler scheme. If $\alpha = \frac{1}{2}$ and $B(U^n)$ is replaced by $(B(U^n)+B(U^{n+1}))/2$, then we obtain the second-order nonlinear Crank-Nicolson scheme.

If we center our schemes in time about time step $t_{n-\alpha/(4+2\alpha)}$, the second-order implicit-explicit schemes can be written as

\[
\frac{U^{n+1} + \alpha U^n - (1 + \alpha)U^{n-1}}{\tau} = \epsilon A \left( (\beta - \frac{\alpha}{2})U^{n+1} + (2 + \frac{3}{2}\alpha - 2\beta)U^n + \beta U^{n-1} \right) \\
+ \left( (2 + \frac{\alpha}{2})B(U^n) + \frac{\alpha}{2}B(U^{n-1}) \right),
\]

where $\alpha$ and $\beta$ are two free parameters. Here we restrict $\beta \geq \frac{\alpha}{2}$ to prevent large truncation error and ensure better stability. Some special cases are classical, e.g.,

- If $(\alpha, \beta) = (-1, 0)$, then we have the Crank-Nicolson/Adams-Bashforth scheme.

\[
\frac{U^{n+1} - U^n}{\tau} = \epsilon A \frac{U^{n+1} + U^n}{2} + \left( \frac{3}{2}B(U^n) - \frac{1}{2}B(U^{n-1}) \right).
\]

- If $(\alpha, \beta) = (-1, \frac{1}{16})$, then we obtain the modified Crank-Nicolson/Adams-Bashforth scheme

\[
\frac{U^{n+1} - U^n}{\tau} = \epsilon A \left( \frac{9}{16}U^{n+1} + \frac{3}{8}U^n + \frac{1}{16}U^{n-1} \right) \\
+ \left( \frac{3}{2}B(U^n) - \frac{1}{2}B(U^{n-1}) \right).
\]

- If $(\alpha, \beta) = (-\frac{4}{3}, 0)$, then we have semi-implicit backward difference formula (BDF)

\[
\frac{3U^{n+1} - 4U^n + U^{n-1}}{2\tau} = \epsilon AU^{n+1} + (2B(U^n) - B(U^{n-1})).
\]

- If $(\alpha, \beta) = (0, 1)$, we have semi-implicit Leap-Frog formula

\[
\frac{U^{n+1} - U^{n-1}}{2\tau} = \epsilon A \frac{U^{n+1} + U^{n-1}}{2} + B(U^n).
\]

\[28\]
2.3.2 First-order IMEX schemes

Taking inner product with $V \in H_0^1(\Omega)$, we have the first-order implicit-explicit method

$$\frac{(U^{n+1} - U^n, V)}{\tau} + \epsilon(\nabla(\alpha U^{n+1} + (1 - \alpha)U^n), \nabla V) + (f(U^n), V) = 0, \quad \forall V \in H_0^1(\Omega).$$

(2.3.11)

**Theorem 2.3.** Consider the scheme (2.3.11) with homogeneous Neumann boundary conditions. If

$$\alpha \geq \frac{1}{2}, \quad \tau \leq \frac{2}{L},$$

(2.3.12)

where $L$ is defined by (2.1.3), then the energy-decay property (1.2.9) holds, i.e.,

$$E(U^{n+1}) \leq E(U^n), \quad \forall n \geq 0.$$  (2.3.13)

**Proof.** Taking $V = U^{n+1} - U^n$ in (2.3.11) and using the identity

$$(\phi - \varphi, 2\phi) = ||\phi||^2 - ||\varphi||^2 + ||\phi - \varphi||^2,$$

yield

$$\frac{1}{\tau}||U^{n+1} - U^n||_0^2 + \left(\alpha - \frac{1}{2}\right)\epsilon||\nabla(U^{n+1} - U^n)||_0^2$$

$$+ \frac{\epsilon}{2}(||\nabla U^{n+1}||_0^2 - ||\nabla U^n||_0^2) + (f(U^n), U^{n+1} - U^n) = 0.$$  (2.3.14)

The above result, together with the Taylor formula

$$F(U^{n+1}) - F(U^n) = f(U^n)(U^{n+1} - U^n) + \int_{U^n}^{U^{n+1}} f'(s)(U^{n+1} - s)ds$$

(2.3.15)

and the definition (1.3.4), give

$$E(U^{n+1}) - E(U^n) + \left(\alpha - \frac{1}{2}\right)\epsilon||\nabla(U^{n+1} - U^n)||_0^2 + \frac{1}{\tau}||U^{n+1} - U^n||_0^2$$

$$= \int_{\Omega} \int_{U^n}^{U^{n+1}} f'(s)(U^{n+1} - s) ds dx.$$  (2.3.16)
This, together with the mean-value theorem and (2.1.3), gives

\[ E(U^{n+1}) - E(U^n) + \left( \alpha - \frac{1}{2} \right) \epsilon \| \nabla(U^{n+1} - U^n) \|^2_0 + \frac{1}{\tau} \| U^{n+1} - U^n \|^2_0 \]

\[ = \frac{1}{2} (f'(\xi^n)(U^{n+1} - U^n), U^{n+1} - U^n) \]

\[ \leq L \int_{\Omega} \int_{U^n}^{U^{n+1}} (U^{n+1} - s)dsdx = \frac{L}{2} \| U^{n+1} - U^n \|^2_0. \] (2.3.17)

The desired result follows from (2.3.17) and the assumption (2.3.12). □ □

It is obvious that as the positive parameter \( \alpha \) increases the scheme has better stability. On the other hand, from (2.3.11) we obtain the first term of truncation error as follows

\[ \left( \frac{1}{2} U^{(2)}(t_n) - \alpha \epsilon AU^{(1)}(t_n) \right) \tau. \]

This implies that larger values of \( \alpha \) may lead to larger truncation errors.

### 2.3.3 Second-order IMEX schemes

Taking inner product with \( V \in H^1_0(\Omega) \) or \( H^1(\Omega) \), we have the second-order implicit-explicit method

\[ (U^{n+1} + \alpha U^n - (1 + \alpha) U^{n-1}, V) \]

\[ \tau \epsilon \left( \nabla ((\beta - \frac{\alpha}{2}) U^{n+1} + (2 + \frac{3}{2}\alpha - 2\beta) U^n + \beta U^{n-1}), \nabla V \right) \]

\[ + \left( (2 + \frac{\alpha}{2}) f(U^n) + \frac{\alpha}{2} f(U^{n-1}), V \right) = 0. \] (2.3.18)

**Theorem 2.4.** In the second-order implicit-explicit scheme (2.3.18), if \( \tau \leq (2 + \alpha)/L \) and either of

\[ \beta \geq 0, \quad -2 < \alpha \leq -1 \] (2.3.19)

or

\[ -\frac{1}{2} < \beta \leq 0, \quad -2 < \alpha \leq 2\beta - 1 \] (2.3.20)

is satisfied, then (2.3.18) is energy-stable in the following sense:

\[ E(U^{n+1}) + \eta_1 \| \nabla(U^{n+1} - U^n) \|^2_0 + \eta_2 \| U^{n+1} - U^n \|^2_0 \]

\[ \leq E(U^n) + \eta_1 \| \nabla(U^n - U^{n-1}) \|^2_0 + \eta_2 \| U^n - U^{n-1} \|^2_0, \] (2.3.21)
for all \( n \geq 0 \), where \( \eta_1, \eta_2 \) are two positive constants.

**Proof.** Taking \( V = U^{n+1} - U^n \) in (2.3.18) and using the Taylor expansion similar to (2.3.15) twice yield:

\[
E(U^{n+1}) - E(U^n) + \frac{\|U^{n+1} - U^n\|_0^2 + (1 + \alpha)(U^{n+1} - U^n, U^n - U^{n-1})}{\tau(2 + \alpha)} \\
+ \frac{(\beta - 1 - \alpha)\epsilon}{2 + \alpha} \|\nabla(U^{n+1} - U^n)\|_0^2 - \frac{\beta\epsilon}{2 + \alpha}(\nabla(U^{n+1} - U^n), \nabla(U^n - U^{n-1})) \\
= \left( \int_{U^n} U^{n+1} f'(s) (U^n - s) ds, 1 \right) - \frac{\alpha}{2(2 + \alpha)} \left( \int_{U^{n-1}} U^n f'(s) ds, U^{n+1} - U^n \right) \\
\leq \frac{L}{2} \|U^{n+1} - U^n\|_0^2 + |\alpha| \frac{L}{2|2 + \alpha|} \|U^{n+1} - U^n\|_0 \|U^n - U^{n-1}\|_0.
\]

(2.3.22)

Using Hölder’s inequality, we have the following inequality

\[
E(U^{n+1}) + C_1 \|\nabla(U^{n+1} - U^n)\|_0^2 + C_2 \|U^{n+1} - U^n\|_0^2 \\
\leq E(U^n) + C_3 \|\nabla(U^n - U^{n-1})\|_0^2 + C_4 \|U^n - U^{n-1}\|_0^2,
\]

(2.3.23)

where

\[
C_1 = \frac{(\beta - 1 - \alpha)\epsilon}{2 + \alpha} - \frac{|\beta|\epsilon}{2|2 + \alpha|}, \quad C_3 = \frac{|\beta|\epsilon}{2|2 + \alpha|}, \\
C_2 = \frac{1}{\tau(2 + \alpha)} - \frac{|1 + \alpha|}{2\tau|2 + \alpha|} - \frac{L}{2} - \frac{|\alpha|L}{4|2 + \alpha|}, \quad C_4 = \frac{|\alpha|L}{4|2 + \alpha|} + \frac{|1 + \alpha|}{2\tau|2 + \alpha|}.
\]

To establish the energy-decay property, we first restrict the choice of parameters by requiring

\[ 0 \leq C_3 \leq C_1 \quad \text{and} \quad 0 \leq C_4 \leq C_2. \]

Clearly, \( C_3 \geq 0 \) and \( C_4 \geq 0 \). Moreover, it is natural to assume that \( 2 + \alpha > 0 \). Simple computation shows that if

\[ \alpha \in (-2, -1] \quad \text{and} \quad \beta \geq 0 \]

(2.3.24)

or

\[ \alpha \in (-2, 2\beta - 1] \quad \text{and} \quad \beta \in (-\frac{1}{2}, 0] \]

(2.3.25)

is satisfies, then we have \( C_1 \geq C_3 \). On the other hand, if \( \tau \leq (2 + \alpha)/L \), then \( C_2 \geq C_4 \).

Setting \((\eta_1, \eta_2) = (C_3, C_4)\) yields the desired result (2.3.21). □
Remark. Note that the discretized energy definition used in Theorem 2.4 (i.e., (3.4.27)) is an $O(\Delta t)$ perturbation of the original definition used in Theorem 4.1. In fact, this seems common for higher order discretizations: when the order of accuracy is increased, the relevant discretized energy has to be modified with some consistent perturbations.

It follows from (2.3.18) that the leading term in the truncation errors is given by
\[
\left( \frac{2+\alpha}{6} U_{tt}(t_n) + (\frac{\alpha}{4} - \beta) \epsilon AU_{tt}(t_n) - \frac{\alpha}{4} f_{tt} \right) \tau^2.
\]
Note that if $(\alpha, \beta) = (-\frac{4}{3}, 0)$, we have the classical semi-implicit BDF as this scheme is obtained by using Taylor expansion at $t = t_{n+1}$. However, if $\alpha \in (-\frac{4}{3}, 2)$, then the resulting schemes are obtained by using Taylor expansion at a time after $t_{n+1}$. Moreover, it is obvious that $\beta > 0$ can enhance the energy stability. Hence, if $\alpha \in (-\frac{4}{3}, 2)$ and $\beta > 0$, better stability is expected. This will be confirmed in the numerical experiment section.

2.3.4 Numerical experiments

In this section, we present some numerical experiments to illustrate the theoretical results obtained in the previous section.

Example 2.3. We first consider
\[
\begin{align*}
  u_t &= \epsilon u_{xx} + u - u^3, \quad x \in [-1, 1], \\
  u(x, 0) &= 0.53x + 0.47 \sin(-1.5\pi x), \\
  u(-1, t) &= -1, \quad u(1, t) = 1.
\end{align*}
\]

with the initial and boundary conditions

For spatial discretization, we use a fourth-order compact scheme to approximate (2.3.26) (see, e.g., [83, 84]):
\[
\left( 1 + \frac{h^2}{12} \delta_x^2 \right) \frac{\partial u_i}{\partial t} = \epsilon \delta_x^2 u_i + \left( 1 + \frac{h^2}{12} \delta_x^2 \right) (u_i - u_i^3),
\]

32
\[ \| \hat{u}_{h,\tau} - u_{h,\tau} \| = 0.1, \frac{\tau}{2}, \frac{\tau}{4}, \frac{\tau}{8}, \frac{\tau}{16} \]

Table 2.7: Example 2.3: numerical accuracy of first-order IMEX scheme with \((\alpha, \beta) = (1, 0)\). Also \(\epsilon = 0.01\) and \(T = 5\).

\[
\begin{array}{cccccc}
\text{Mesh} & \tau = 0.1 & \tau/2 & \tau/4 & \tau/8 & \tau/16 \\
\| \hat{u}_{h,\tau} - u_{h,\tau} \| & 3.0529e-3 & 1.5742e-3 & 7.9852e-4 & 4.0100e-4 & 1.9972e-5 \\
\text{Rate} & / & 0.95552 & 0.97921 & 0.99378 & 1.0056 \\
\end{array}
\]

Table 2.7: Example 2.3: Numerical accuracy of second-order IMEX scheme with \((\alpha, \beta) = (-1.5, 1)\). Also \(\epsilon = 0.01\) and \(T = 5\).

\[
\begin{array}{cccccc}
\text{Mesh} & \tau = 0.1 & \tau/2 & \tau/4 & \tau/8 & \tau/16 \\
\| \hat{u}_{h,\tau} - u_{h,\tau} \| & 1.2588e-4 & 3.5477e-5 & 9.3755e-6 & 2.4071e-6 & 6.0956e-7 \\
\text{Rate} & / & 1.8271 & 1.9199 & 1.9616 & 1.9814 \\
\end{array}
\]

where \(\delta^2_x\) denotes the second-order central difference operator.

To verify the numerical accuracy, we take the numerical solution \(\hat{u}_{h,\tau}\) obtained using the first-order and second-order implicit-explicit scheme with \(h = 1/32\) and \(\tau = 10^{-3}\) as the exact solution as compared with the corresponding coarse time-stepping approximation. The \(L^2\)-norm error and convergence rate for the first-order IMEX scheme with \((\alpha, \beta) = (1, 0)\) are shown in Table 2.7, while those for the second-order IMEX scheme with \((\alpha, \beta) = (-1.5, 1)\) are shown in Table 2.8. It is observed that above schemes give predicted orders of accuracy in time.

Figure 2.2 shows the time evolution of the Allen-Cahn equation for different time steps. It is observed from Fig. 2.2(a) that the initial hump is metastable and disappears before \(t = 40\) as \(\tau = 0.1\). However, the initial hump is metastable and disappears near \(t = 45\) if a larger time-step \(\tau = 0.5\) is used. In both cases we choose \((\alpha, \beta) = (0.5, 1)\). This indicates that the initial hump delays as \(\tau\) increases.

In [75], Kassam and Trefethen use the exponential time-differencing fourth-order Runge-Kutta method for time-stepping. Their results suggest that the initial hump...
disappears near $t = 45$, which is comparable to our coarse time-step results with $	au = 0.5$.

Figure 2.2: Time evolution for Example 2.3. (a). $\tau = 0.1$; in this case the initial hump is metastable and disappears before $t = 40$; (b). $\tau = 0.5$; in this case the initial hump disappears near $t = 45$.

The energy evolution for Example 2.3 solved by our first-order scheme with different parameters are shown in Figs. 2.3 and 2.4. In Fig. 2.3, we fix the parameters $\alpha$ and $\beta$ ( $\alpha = 1$ or $2$ and $\beta = 0$). It is observed that the accuracy is improved as $\tau$ decreases. In Fig. 2.4, we fix $\tau = 0.1$ and vary $\alpha$, and it is observed that the accuracy is affected if large values of $\alpha$ are used.

The results using second-order implicit-explicit scheme with different parameters are shown in Fig. 2.5, where we fix $\beta = 0$ and $\tau = 0.5$ and change $\alpha$. In this case, it follows from Theorem 2.4 if $\alpha$ is not within the interval $(-2, -1]$ the energy stability may not be guaranteed. To test this, we choose $\alpha = -0.99$ and $-2.01$ (both are out of the $(-2, -1]$) and in both cases the energy curves violate the energy-decay property.

It is observed in Figs. 2.3-2.5 that nonlinear energy stability is preserved if the parameters satisfy the conditions stated in Theorems 2.3 and 2.4.
Example 2.4. Consider 2D problem (1.2.1) with \( f(u) = u - u^3 \) and with the initial condition

\[
u_0(x, y) = 0.05 \sin(x) \sin(y), \quad (x, y) \in [0, 2\pi] \times [0, 2\pi],
\]

The parameter \( \epsilon \) will be chosen as 0.01. Firstly, the physical domain is partitioned with a \( N \times N \) uniform grid. To test the numerical accuracy, we take the numerical solution obtained using the second-order implicit-explicit scheme (2.3.6) with \( N = 60 \) and \( \tau = 10^{-3} \) as the exact solution. The \( L^2 \)-norm error for \( (\alpha, \beta) = (-1/5, 1) \) and \( T = 1.2 \) is shown in Table 2.9, from which it is clearly observed that above scheme gives desired (second) order of accuracy in time.
Figure 2.5: Example 2.3: the energy evolution using second-order scheme (2.3.6) with \( \tau = 0.5 \) and \( \beta = 0 \).

<table>
<thead>
<tr>
<th>Mesh</th>
<th>( \tau = 0.08 )</th>
<th>( \tau/2 )</th>
<th>( \tau/4 )</th>
<th>( \tau/8 )</th>
<th>( \tau/16 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( | \hat{u}<em>{\tau} - u</em>{\tau} | )</td>
<td>1.6795e-2</td>
<td>4.7255e-3</td>
<td>1.2497e-3</td>
<td>3.1904e-4</td>
<td>7.8431e-5</td>
</tr>
<tr>
<td>Rate</td>
<td>/</td>
<td>1.8295</td>
<td>1.9189</td>
<td>1.9697</td>
<td>2.0242</td>
</tr>
</tbody>
</table>

Table 2.9: Example 2.4: rate of convergence in time for scheme (2.3.6) for the 2D Allen-Cahn equation.

We now study the effect of parameters for energy stability. Firstly, we choose \((\alpha, \beta, \tau) = (-4/3, 0, 0.01)\), i.e., the classical BDF method, to obtain the ‘accurate’ energy curve in Fig. 2.6(a). We then fix \( \tau = 0.1 \) and \( \beta = 0 \) and change \( \alpha \). It is observed in Fig. 2.6(b) if the values of \( \alpha \) are chosen out of the \((-2, -1]\) (as given in Theorem 2.4), then the energy curves blow up within a finite time.

Furthermore, Fig. 2.6(b) shows the energy curves for \( \tau = 0.2, \alpha = -4/3 \) and variable \( \beta \). In this case, \((\alpha, \beta) = (-3/4, 1)\) and \((-3/4, -0.5)\) do not satisfy the conditions (2.3.19) or (2.3.20) and the corresponding energy curves also blow up. For the case of \( \beta = 0 \), the condition (2.3.19) is satisfied and the corresponding energy decays are obtained.
Figure 2.6: Example 2.4: the energy evolution with second-order scheme (2.3.6) as (a): fix $\beta = 0$, $\tau = 0.1$, and (b): fix $\alpha = -3/4$, $\tau = 0.2$.

2.4 Concluding remarks

We mainly focus on the nonlinear energy stability for Allen-Cahn equations and Cahn-Hilliard equations. In the first part of this chapter, we apply the stabilized Crank-Nicolson/Adams-Bashforth scheme for approximating both Allen-Cahn equations and Cahn-Hilliard equations. For the spatial discretization, we use the standard conforming finite element method. We provide the values range of stabilized parameters to guarantee energy bounded. Moreover, optimal error estimate of the proposed second-order scheme are derived in details.

Second part, we investigate the first- and second-order implicit-explicit schemes with parameters for solving the Allen-Cahn equation. We analyze the relationship between the energy stability and range of free parameters for both the first-order and second-order schemes. We also believe these multi-step implicit-explicit schemes can be applied for simulating Cahn-Hilliard equations and thin film models.
Chapter 3

Maximum principle for the Allen-Cahn-type equations

Besides the nonlinear energy stability of Allen-Cahn equations, another important property is the maximum principle. More specifically, if the initial values and boundary conditions are both bounded by 1, the entire solution of Allen-Cahn equations is uniformly bounded by 1. The energy stability has been studied extensively including the previous chapter of this thesis, and, up to author’s knowledge, rare literatures focus on the maximum principle. In this chapter, we are devoted to establishing the numerical maximum principle via several numerical schemes for several Allen-Cahn-type equations. Three Allen-Cahn-type equations are into our consideration, that is, standard Allen-Cahn equation, generalized Allen-Cahn equations and fractional-in-space Allen-Cahn equations. More details are given in the following three subsections respectively.

3.1 Preliminaries

In this section we give some useful preliminaries for the finite difference discretization for both the standard Laplace operator and the Riesz fractional Laplace operator. Next we will give the concrete form of the discrete matrix of these two kinds of Laplace operators subjected with homogeneous Dirichlet boundary conditions.
First, the discrete matrix of the standard Laplace operator in 1D is given by

\[
D_h^{(1)} = \Lambda_h =: \frac{1}{h^2} \begin{bmatrix}
-2 & 1 \\
1 & -2 & 1 \\
& \ddots & \ddots & \ddots \\
& 1 & -2 & 1 \\
1 & -2
\end{bmatrix}_{N \times N},
\]

where \( h \) is the width of an 1D uniform mesh. By using the notation of the Kronecker tensor product, we can obtain the discrete matrix in 2D:

\[
D_h^{(2)} = I \otimes \Lambda_h + \Lambda_h \otimes I,
\]

where \( I \) is the \( N \times N \) identity matrix. Similarly, the discrete matrix of 3D case can be represented as

\[
D_h^{(3)} = I \otimes I \otimes \Lambda_h + I \otimes \Lambda_h \otimes I + \Lambda_h \otimes I \otimes I.
\]

Now we turn our attention to the Riesz fractional Laplace operator. The fractional Laplacian operator in one-space dimension is defined by the Riesz fractional derivative

\[
-(-\Delta)^\alpha u = -(-\Delta)^\alpha_{x} u =: \frac{1}{-2 \cos \frac{\pi \alpha}{2}} (aD_x^\alpha u + xD_y^\alpha u),
\]

where the left and right Riemann-Liouville fractional derivatives are defined as

\[
aD_x^\alpha u = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_a^x \frac{u(\xi)}{(x-\xi)^{\alpha-1}},
\]

\[
xD_y^\alpha u = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_x^b \frac{u(\xi)}{(x-\xi)^{\alpha-1}}.
\]

The fractional Laplacian operators in 2D and 3D can be defined similarly. For example, the 3D operator is defined as

\[
-(-\Delta)^\alpha u(x, y, z) = \left\{ \left[ -(-\Delta)^\alpha_x u \right] + \left[ -(-\Delta)^\alpha_y u \right] + \left[ -(-\Delta)^\alpha_z u \right] \right\} u(x, y, z).
\]

We will adopt the finite difference approach in [66] to discretize the fractional Laplacian operator \(-(-\Delta)^\alpha\). To begin with, we denote \( D_h \) as the discrete matrix
of the factional Laplacian operator. In particular, the discrete matrix of $\alpha D_x^\alpha$ with homogeneous Dirichlet boundary conditions on interval $[0, L]$ in one-space dimension is given by

$$A = \frac{1}{h^\alpha} \begin{bmatrix} \omega_0^{(\alpha)} & \omega_1^{(\alpha)} \\ \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} \\ \vdots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \ddots \\ \omega_{N-1}^{(\alpha)} & \ldots & \ldots & \omega_0^{(\alpha)} \\ \omega_N^{(\alpha)} & \omega_{N-1}^{(\alpha)} & \ldots & \omega_2^{(\alpha)} & \omega_1^{(\alpha)} \end{bmatrix} =: \frac{1}{h^\alpha} M,$$

where

$$\omega_0^{(\alpha)} = \frac{\alpha}{2}, \quad \omega_1^{(\alpha)} = \frac{2-\alpha^2}{2} < 0, \quad \omega_2^{(\alpha)} = \frac{\alpha(\alpha^2-\alpha-4)}{4},$$

$$1 \geq \omega_0^{(\alpha)} \geq \omega_3^{(\alpha)} \geq \omega_4^{(\alpha)} \geq \ldots \geq 0, \quad \sum_{k=0}^\infty \omega_k^{(\alpha)} = 0,$$

and $h$ is the mesh size in space. Note that the discrete matrix of $\alpha D_x^\alpha$ is $A^T$. Defining

$$D = M + M^T$$

produces the discrete matrix of the fractional Laplacian operator in one-space dimension:

$$D_h^{(1)} = \frac{1}{-2h^\alpha \cos \frac{\pi \alpha}{2}} D.$$  \hspace{1cm} (3.1.9)

Using the Kronecker tensor product notation, we can obtain the corresponding discrete matrix in two space dimension

$$D_h^{(2)} = \frac{1}{-2h^\alpha \cos \frac{\pi \alpha}{2}} (I \otimes D + D \otimes I),$$

$$D_h^{(3)} = \frac{1}{-2h^\alpha \cos \frac{\pi \alpha}{2}} (I \otimes I \otimes D + I \otimes D \otimes I + D \otimes I \otimes I).$$

Following we give three lemmas which can be satisfied by the discrete matrix of both the standard Laplace operator and the Riesz fractional Laplace operator independent on the dimensions.
Lemma 3.1. If $D_h^{(d)}$, $d = 1, 2, 3$, is the discrete matrix of both standard Laplace operator and the Riesz fractional Laplace operator. Then $D_h = D_h^{(d)}$ satisfies the following properties:

- $D_h$ is symmetric;
- $D_h$ is negative definite, i.e., $U^T D_h U < 0$, for any $U \in \mathbb{R}^N$;
- The elements of $D_h = (b_{ij})$ satisfy:

$$b_{ii} = -b < 0 \text{ and } b \geq \max_i \sum_{j \neq i} |b_{ij}|. \quad (3.1.12)$$

Proof. It is easy to check the above three properties satisfied by the discrete matrix of both standard Laplace operator independent on the dimensions. So we only prove this lemma for the fractional case. From the definitions (3.1.9)-(3.1.11), it is obvious that if $D$ in (3.1.8) satisfies the three properties above so does $D_h$. Consequently, we only need to check whether $D$ satisfies the three properties. First, it follows from the definition $D = M + M^T$ that $D$ is symmetric. Moreover, it can be easily verified that $D = (d_{ij})$ is of the form

$$D = \begin{bmatrix}
2\omega_1^{(\alpha)} & \omega_0^{(\alpha)} + \omega_2^{(\alpha)} & \ldots & \omega_{N-1}^{(\alpha)} & \omega_N^{(\alpha)} \\
\omega_1^{(\alpha)} + \omega_2^{(\alpha)} & 2\omega_1^{(\alpha)} & \omega_0^{(\alpha)} + \omega_2^{(\alpha)} & \ldots & \omega_{N-1}^{(\alpha)} \\
\vdots & \omega_0^{(\alpha)} + \omega_2^{(\alpha)} & 2\omega_1^{(\alpha)} & \ddots & \vdots \\
\omega_0^{(\alpha)} + \omega_2^{(\alpha)} & \ldots & \ddots & \ddots & \omega_0^{(\alpha)} + \omega_2^{(\alpha)} \\
\omega_N^{(\alpha)} & \omega_{N-1}^{(\alpha)} & \ldots & \omega_0^{(\alpha)} + \omega_2^{(\alpha)} & 2\omega_1^{(\alpha)} \\
\end{bmatrix}_{N \times N} \quad (3.1.13)$$

Since $1 < \alpha \leq 2$, we have

$$d_{ii} = 2\omega_1^{(\alpha)} = 2 - \alpha - \alpha^2 \leq 0. \quad (3.1.14)$$

Observe that

$$\omega_0^{(\alpha)} + \omega_2^{(\alpha)} = \frac{\alpha}{2} + \frac{\alpha(\alpha^2 + \alpha - 4)}{4} = \frac{\alpha(\alpha^2 + \alpha - 2)}{4} \geq 0$$
and $\omega_3^{(\alpha)} \geq \omega_4^{(\alpha)} \geq \ldots \geq 0$. We then obtain that $d_{ij} \geq 0$, $i \neq j$. Furthermore, it follows from (3.1.7) that
\[
-\omega_1^{(\alpha)} > \omega_0^{(\alpha)} + \sum_{k=2}^{N} \omega_k^{(\alpha)} \quad \text{for } 1 < \alpha < 2,
\]
\[
-\omega_1^{(\alpha)} = \omega_0^{(\alpha)} + \sum_{k=2}^{\infty} \omega_k^{(\alpha)} \quad \text{for } \alpha = 2.
\]
Consequently,
\[
-d_{ii} = -2\omega_1^{(\alpha)} \geq 2\omega_0^{(\alpha)} + 2\sum_{k=2}^{N} \omega_k^{(\alpha)} \geq \max_i \sum_{i \neq j} |d_{ij}|. \quad (3.1.15)
\]
This verifies (3.1.12), which implies that $D$ is negative diagonally dominated and hence negative definite. This completes the proof. \qed

**Lemma 3.2.** Let $B$ be a real $N \times N$ matrix and $A = aI - B$ with $a > 0$. If $B = (b_{ij})$ satisfies (3.1.12), then
\[
\|Av\|_{\infty} \geq a\|v\|_{\infty}, \quad \|Av + c(v)^3\|_{\infty} \geq a\|v\|_{\infty} + c\|v\|_{\infty}^3, \quad (3.1.16)
\]
where $c > 0$ and $v \in \mathbb{R}^N$.

**Proof.** Suppose $\|v\|_{\infty} = |v_p|$. Then $|v_p| \geq |v_j|$ for all $1 \leq j \leq N$. To simplify the notation, denote
\[
s = Av, \quad t = Av + c(v)^3. \quad (3.1.17)
\]
Then the $p$th components of $s$ and $t$ are
\[
s_p = av_p - \sum_{j=1}^{N} b_{pj}v_j, \quad t_p = av_p + cv_p^3 - \sum_{j=1}^{N} b_{pj}v_j. \quad (3.1.18)
\]
Obviously, $av_p$ and $cv_p^3$ have the same signs. Next we will check both $av_p$ and $-\sum_{j=1}^{N} b_{pj}v_j$ have the same sign. This can be verified by
\[
\begin{align*}
av_p \cdot \left(-\sum_{j=1}^{N} b_{pj}v_j\right) & = av_p \left(-b_{pp}v_p - \sum_{j \neq p} b_{pj}v_j\right) = a \left(bv^2_p - \sum_{j \neq p} b_{pj}v_jv_p\right) \\
& \geq a \left(b|v_p|^2 - \sum_{j \neq p} |b_{pj}||v_j||v_p|\right) \geq a \left(b|v_p|^2 - \sum_{j \neq p} |b_{pj}||v_p|^2\right) \\
& \geq a \left(b - \sum_{j \neq p} |b_{pj}|\right)|v_p|^2 \geq 0. \quad (3.1.19)
\end{align*}
\]
Therefore $av_p$, $cv^3_p$ and $-\sum_{j=1}^{N} b_{pj} v_j$ are positive or negative simultaneously. Consequently,

$$|s_p| \geq a|v_p| = a\|v\|_{\infty}, \quad |t_p| \geq a|v_p| + c|v_p|^3 = a\|v\|_{\infty} + c\|v\|_{\infty}^3.$$  \hfill (3.1.20)

Using the facts $\|s\|_{\infty} \geq |s_p|$ and $\|t\|_{\infty} \geq |t_p|$ yields the desired estimates (3.1.16). \hfill \Box

**Lemma 3.3.** Let $B \in \mathbb{R}^{N \times N}$ and $A = aI - B$, where $a > 0$. If $B = (b_{ij})$ is a negative diagonally dominant (NDD) matrix, i.e.

\begin{align*}
i) & \quad b_{ii} \leq 0, \\
\text{ii}) & \quad b_{ii} + \sum_{j \neq i} |b_{ij}| \leq 0, \quad \forall i,
\end{align*}  \hfill (3.1.21)

then

$$\|A^{-1}\|_{\infty} \leq \frac{1}{a}. \hfill (3.1.22)$$

**Proof.** If $B$ is a zero matrix, the conclusion holds obviously. Otherwise, we denote

$$b = \max_i (-b_{ii}) > 0.$$  \hfill (3.1.23)

Then we rewrite $A$ as

$$A = (a + b)I - (bI + B) := (a + b)(I - sC),$$  \hfill (3.1.24)

where $s = \frac{b}{a+b} < 1$, and matrix $C = I + \frac{1}{b}B := (c_{ij})$. Thus

\begin{align*}
\|C\|_{\infty} &= \max_i \sum_j |c_{ij}| = \max_i \left( 1 + \frac{b_{ii}}{b} + \frac{1}{b} \sum_{j \neq i} |c_{ij}| \right) \\
&= \max_i \left( 1 + \frac{1}{b} (b_{ii} + \sum_{j \neq i} |c_{ij}|) \right) \leq 1.
\end{align*}  \hfill (3.1.25)

Then we have

$$\rho(sC) = s \rho(C) \leq s < 1,$$  \hfill (3.1.26)

where $\rho(C)$ is the spectral radius of matrix $C$. As the inverse of $I - sC$ can be represented by the power series of $sC$, we have

$$\|A^{-1}\|_{\infty} = \left\| \frac{1}{a+b} \sum_{p=0}^{\infty} (sC)^p \right\|_{\infty} \leq \frac{1}{a+b} \sum_{p=0}^{\infty} s^p \|C\|_{\infty}^p \leq \frac{1}{a+b} \cdot \frac{1}{1-s} = \frac{1}{a},$$  \hfill (3.1.27)

where in the last step we have used the definition $s = \frac{b}{a+b} < 1$. \hfill \Box
We close this section by defining the discrete energy of the continuum free energy. Subjected with the periodic or homogeneous Neumann/Dirichlet boundary conditions, we have

\[
E(u) = \int_{\Omega} \left( \frac{1}{2} \epsilon^2 |\nabla u|^2 + F(u) \right) dx = \int_{\Omega} \left( -\frac{1}{2} \epsilon^2 u \Delta u + F(u) \right) dx.
\]

The discrete energy function can be represented by the discrete Laplace operator \(D_h\) given below

\[
E_h(U) = h^d \left( -\frac{\epsilon^2}{2} U^T D_h U + \sum_{i=1}^{N} F(U_i) \right),
\]

where \(d\) is the number of dimension.

### 3.2 Discrete maximum principle for the Allen-Cahn equation

This section is concerned with the numerical maximum principle of the Allen-Cahn equation

\[
\frac{\partial u}{\partial t} = \epsilon^2 \Delta u - f(u), \quad x \in \Omega, \quad t \in (0, T],
\]

with the initial condition

\[
u(x, 0) = u_0(x), \quad x \in \overline{\Omega},
\]

We consider the commonly used double well potential which gives

\[
f(u) = u^3 - u.
\]

The most conventional approach for solving (3.2.1) is to use the standard implicit-explicit scheme in time and central finite difference in space:

\[
\frac{U^{n+1} - U^n}{\tau} + ((U^n)^3 - U^n) = \epsilon^2 D_h U^{n+1},
\]

where \(\tau\) denotes the time stepsize, \(U^n\) represents the vector of numerical solution at the \(t = t_n\) level, and \((U^n)^3 = ((U^n_1)^3, (U^n_2)^3, \ldots, (U^n_N)^3)^T\).
3.2.1 Discrete maximum principle and discrete energy stability

**Theorem 3.1.** Consider the Allen-Cahn problem (3.2.1)-(3.2.3) with periodic or homogeneous Neumann/Dirichlet boundary conditions. If the initial value is bounded by 1, i.e., \( \max_{x \in \Omega} |u_0(x)| \leq 1 \), then the fully discrete scheme (3.2.4) is also bounded by 1 in the sense that

\[
\|U^n\|_\infty \leq 1 \tag{3.2.5}
\]

for all \( n > 0 \) provided that the time stepsize satisfies \( 0 < \tau \leq \frac{1}{2} \).

**Proof.** We prove our claim by induction. Obviously, \( \|U^0\|_\infty \leq \|u_0\| \leq 1 \). We assume \( \|U^m\|_\infty \leq 1 \) and will verify the result is true for \( U^{m+1} \). It follows from the scheme (3.2.4) that

\[
U^{m+1} = (I - \tau \epsilon^2 D_h)^{-1}(U^m + \tau (U^m - (U^m)^3)). \tag{3.2.6}
\]

Using Lemma 3.1 gives

\[
\|(I - \tau \epsilon^2 D_h)^{-1}\|_\infty \leq 1. \tag{3.2.7}
\]

Note that each element of \( U^m + \tau (U^m - (U^m)^3) \) is of the form \( g(x) = x + \tau (x - x^3) \). It can be verified that if \( 0 < \tau \leq \frac{1}{2} \) then \( g'(x) \geq 0 \) for \( x \in [-1,1] \). This gives that

\[
\max_{|x| \leq 1} g(x) = g(1) = 1; \quad \min_{|x| \leq 1} g(x) = g(-1) = -1,
\]

which implies that \( \|g\|_\infty = 1 \). Consequently, we can conclude that

\[
\|U^m + \tau (U^m - (U^m)^3)\|_\infty \leq 1 \quad \text{if} \quad \|U^m\|_\infty \leq 1. \tag{3.2.8}
\]

This, together with (3.2.6) and (3.2.7), gives

\[
\|U^{m+1}\|_\infty \leq \|(I - \tau \epsilon^2 D_h)^{-1}\|_\infty \cdot \|U^m + \tau (U^m - (U^m)^3)\|_\infty \leq 1. \tag{3.2.9}
\]

This completes the proof. \( \square \)
Theorem 3.2. Under the same conditions in Theorem 3.1, the numerical solutions obtained by the scheme (3.2.4) satisfies the discrete energy-decreasing property:

\[ E_h(U^{n+1}) \leq E_h(U^n), \quad (3.2.10) \]

provided that the time stepsize satisfies \( 0 < \tau \leq \frac{1}{2} \).

Proof. Taking the difference of the discrete energy between two consecutive time levels gives

\[ E_h(U^{n+1}) - E_h(U^n) = \frac{h^d}{4} \sum_{i=1}^{N} \left[ ((U_i^{n+1})^2 - 1)^2 - ((U_i^n)^2 - 1)^2 + \frac{\epsilon^2 h^d}{2} \left( (U_i^{n+1})^T D_h U^{n+1} - (U_i^n)^T D_h U^n \right) \right]. \quad (3.2.11) \]

Note that for all \( a, b \in [-1, 1] \):

\[ (b^3 - b)(a - b) + (a - b)^2 \geq \frac{1}{4}[(a^2 - 1)^2 - (b^2 - 1)^2]. \quad (3.2.12) \]

It follows from Theorem 3.1 that \( ||U^{n+1}||_\infty, ||U^n||_\infty \leq 1 \) with \( 0 < \tau \leq \frac{1}{2} \). This fact, together with (3.2.11), gives

\[ E_h(U^{n+1}) - E_h(U^n) \leq \frac{h^d}{4} \sum_{i=1}^{N} \left[ ((U_i^n)^3 - U_i^n)(U_i^{n+1} - U_i^n) + (U_i^{n+1} - U_i^n)^2 \right] + \frac{\epsilon^2 h^d}{2} \left( (U_i^{n+1})^T D_h U^{n+1} - (U_i^n)^T D_h U^n \right). \quad (3.2.13) \]

Taking \( L^2 \) inner product for (3.2.4) with \( (U_i^{n+1} - U_i^n)^T \) yields

\[ \sum_{i=1}^{N} \left[ ((U_i^n)^3 - U_i^n)(U_i^{n+1} - U_i^n) + \frac{1}{\tau}(U_i^{n+1} - U_i^n)^2 \right] = \epsilon^2 (U^{n+1} - U^n)^T D_h U^{n+1}. \quad (3.2.14) \]

Since the discrete Laplace operator \( D_h \) is symmetric, we can rewrite the right-hand side of (3.2.6) as

\[ \epsilon^2 (U^{n+1} - U^n)^T D_h U^{n+1} = \frac{\epsilon^2}{2} ((U^{n+1})^T D_h U^{n+1} - (U^n)^T D_h U^n) + \frac{\epsilon^2}{2} ((U^{n+1} - U^n)^T D_h (U^{n+1} - U^n)). \quad (3.2.15) \]
Consequently, combining (3.2.13)-(3.2.15) gives

\[ E_h(U^{n+1}) - E_h(U^n) - \frac{\epsilon^2 h^d}{2} (U^{n+1} - U^n)^T D_h (U^{n+1} - U^n) \leq 0. \]  

(3.2.16)

Since \( D_h \) is negative semidefinite, the desired result (3.2.10) follows from the above inequality.

### 3.2.2 Stabilized semi-implicit schemes

It is shown in the previous section that the commonly used scheme (3.2.4) is conditionally stable. To obtain an unconditionally stable semi-implicit scheme, we can add an extra stabilized term which is consistent with the truncation error. For example, we can follow [43]

\[ \frac{U^{n+1} - U^n}{\tau} + ((U^n)^3 - U^n) + \beta (U^{n+1} - U^n) = \epsilon^2 D_h U^{n+1}, \]  

(3.2.17)

where \( \beta > 0 \) is a constant.

**Theorem 3.3.** Consider the Allen-Cahn problem (3.2.1)-(3.2.3) with periodic or homogeneous Neumann/Dirichlet boundary conditions. If the initial value is bounded by 1, i.e., \( \max_{x \in \Omega} |u_0(x)| \leq 1 \), then the numerical solutions obtained by the scheme (3.2.17) satisfy

\[ ||U^n||_{\infty} \leq 1, \quad E_h(U^{n+1}) \leq E_h(U^n) \]  

(3.2.18)

provided that

\[ \beta + \frac{1}{\tau} \geq 2, \]  

(3.2.19)

where the discrete energy \( E_h \) is defined by (3.1.29). In particular when \( \beta \geq 2 \), the numerical scheme (3.2.17) is unconditionally pointwise stable and energy stable.

**Proof.** The proof is similar to that of Theorems 3.1 and 3.2, and will be omitted here. 

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3.2.3 Error analysis

In this sub-section, we will establish error estimates for the fully discrete formulation of the standard implicit-explicit scheme (3.2.4). The error $U^n$ is defined as

$$E^n = U(t_n) - U^n,$$ (3.2.20)

where $U(t_n)$ is the exact solution of (3.2.1)-(3.2.3).

First, we define the local truncation error $T^n$ for the scheme (3.2.4) by

$$T^n = (I - \tau \epsilon^2 D_h)U(t_n) - (U(t_{n-1}) + \tau(U(t_{n-1}) - (U(t_{n-1}))^3)).$$ (3.2.21)

We assume the solution $U(t)$ is sufficient smooth and the scheme (3.2.4) is consistent. Hence, it follow that

$$||T^j||_\infty \leq c \tau \eta \quad \text{for} \quad j \leq n,$$ (3.2.22)

where $\eta = \tau + h^2$ and $c = c(t_n)$ is a positive function of $t$ which may depend on $U(t)$ but not on $\tau$ or $h$. Based on the smoothness and consistency assumption, we then have

**Theorem 3.4.** Under the same conditions in Theorem 3.1, assume that solution $u(x, t)$ is sufficient smooth and the scheme (3.2.4) is consistent in the sense of (3.2.22). We have the following error estimate

$$||E^n||_\infty \leq e^{\kappa t_n}(\tau + h^2),$$ (3.2.23)

where $\kappa = \max\{c, 2\}$.

**Proof.** We rewrite the scheme (3.2.4) as

$$(I - \tau \epsilon^2 D_h)U^n = U^{n-1} + \tau(U^{n-1} - (U^{n-1})^3).$$ (3.2.24)

Subtracting (3.2.24) from (3.2.21) obtains

$$(I - \tau \epsilon^2 D_h)E^n = E^{n-1} + \tau[(U(t_{n-1}) - (U(t_{n-1}))^3) - (U^{n-1} - (U^{n-1})^3)] + T^n.$$ (3.2.25)
From the fundamental inequality

\[ |(a - a^3) - (b - b^3)| \leq 2|a - b| \quad \text{for} \quad \forall a, b \in [-1, 1], \quad (3.2.26) \]

it is easy to derive

\[ ||(U(t_{n-1}) - (U(t_{n-1}))^3) - (U^{n-1} - (U^{n-1})^3)||_\infty \leq 2||E^{n-1}||_\infty, \quad (3.2.27) \]

due to both \( U(t_j) \) and \( U^j \) lying in \([-1, 1]\) for \( j \leq n \). Combining (3.2.21) and (3.2.27) and using Lemma 3.1, we have from (3.2.25)

\[ ||E^n||_\infty \leq (1 + \kappa \tau)||E^{n-1}||_\infty + \kappa \tau \eta, \quad (3.2.28) \]

where \( \kappa = \max\{c, 2\} \). By induction it follows

\[ ||E^n||_\infty \leq (1 + \kappa \tau)^n ||E^0||_\infty + \kappa \tau \eta \sum_{j=0}^{n-1} (1 + \kappa \tau)^j \quad (3.2.29) \]

\[ \leq e^{\kappa \tau n} ||E^0||_\infty + \kappa \eta, \quad (3.2.30) \]

which is the desired result (3.2.23).

\[ \Box \]

### 3.2.4 Numerical tests

In this section, we present some numerical experiments to verify the theoretical results obtained in the previous sections. Since our analysis is independent of dimensions, for simplicity we only consider one-dimensional problems for (3.2.1) with homogeneous Neumann boundary condition.

**Example 3.1.** The initial condition is chosen as

\[ u_0(x) = 0.9 \times \text{rand}(\cdot) + 0.05, \]

where "\( \text{rand}(\cdot) \)" represents a random number on each point in \([0, 1]\). The parameter \( \epsilon^2 \) is 0.001, the computation domain is \([0, 1]\) and the mesh size in space is \( h = 0.01 \).
Figure 3.1: Energy curves for the scheme (3.2.4) with different time steps $\tau = 0.5, 0.75, 1, 3$.

Figure 3.2: Maximum values for the scheme (3.2.4) with different time steps $\tau = 0.5, 0.75, 1, 3$.

We first consider the standard implicit-explicit scheme (3.2.4). Fig. 3.1 plots the energy curves for several values of $\tau$, and it is found that the energy blows up
Figure 3.3: Energy curves and maximum values for (3.2.17) with $\beta = 1$ and time steps $\tau = 0.5, 1, 3$.

Figure 3.4: Same as Fig. 3.3, except with $\beta = 2$.

quickly when $\tau = 3$. Fig. 3.2 plots the maximum solution values against time, and the numerical results are in excellent agreement of our theoretical analysis. More precisely, the maximum principle is preserved for $\tau = 0.5$ and is violated when $\tau = 3$.
0.75, 1, 3.

Fig. 3.3 gives the numerical results obtained using the modified scheme (3.2.17) with \( \beta = 1 \). Several time stepsizes \( \tau \) are used. It is seen when the requirement \( \beta + 1/\tau \geq 2 \) is not satisfied with \( \beta = 1 \) and \( \tau = 3 \) the maximum principle is violated. Finally, we change \( \beta \) from 1 to 2 and it is observed from Fig. 3.4 that the corresponding scheme becomes unconditionally stable. This is in good agreement with the results of Theorem 3.3.

### 3.3 Discrete maximum principle for the generalized Allen-Cahn equation

In this section, we study the numerical maximum principle of the generalized Allen-Cahn equation:

\[
\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = M(u)(\epsilon \Delta u - \frac{1}{\epsilon}F'(u)), \quad x \in \Omega, t \in (0, T], \quad (3.3.1)
\]

\[
u(x, 0) = u_0(x), \quad x \in \bar{\Omega}, \quad (3.3.2)
\]

subjected to a suitable boundary condition such as periodic boundary conditions, homogeneous Neumann boundary conditions or homogeneous Dirichlet boundary conditions. \( \Omega \) is a bounded domain in \( \mathbb{R}^d \) \((d = 1, 2, 3)\), \( M(u) \) is the mobility function, \( F(u) \) is a potential function, and \( \mathbf{v}(\cdot, t) \) is a given velocity field.

In the usual case, the free energy function \( F(u) \) has a double well form with minima at \( \beta \) and \( -\beta \) where \( \beta \) satisfies

\[
F'(\beta) = F'(-\beta) = 0. \quad (3.3.3)
\]

Moreover, the \( F'(u) \) satisfies the following conditions

\[
F'(u) < 0, \quad \forall \beta \in (-\infty, -\beta); \quad F'(u) > 0, \quad \forall \beta \in (\beta, \infty). \quad (3.3.4)
\]

The mobility function is assumed to be non-negative, i.e.,

\[
M(u) \geq 0, \quad \forall \beta \in [-\beta, \beta]. \quad (3.3.5)
\]
Under the conditions (3.3.3 - 3.3.5), the Allen-Cahn equation (3.3.1) satisfies a maximum principle. Specifically, if the initial value and the boundary conditions are bounded by $\beta$, the entire solution to the Allen-Cahn equation is also bounded by $\beta$.

In this section, we will mainly focus on establishing the maximum principle for finite difference approximations to the generalized Allen-Cahn equations with potential satisfying (3.3.3)-(3.3.4) and mobility satisfying (3.3.5).

### 3.3.1 The semi-discrete semi-implicit scheme

First, we consider the standard linearized semi-implicit scheme

$$\frac{u^{n+1} - u^n}{\tau} + v^{n+1} \cdot \nabla u^{n+1} = M(u^n)(\epsilon \Delta u^{n+1} - \frac{1}{\epsilon} F'(u^n)), \quad (3.3.6)$$

which can be rewritten as

$$u^{n+1} + \tau v^{n+1} \cdot \nabla u^{n+1} - \tau \epsilon M(u^n) \Delta u^{n+1} = u^n - \frac{\tau}{\epsilon} M(u^n) F'(u^n), \quad (3.3.7)$$

where $u^n, v^n$ are approximations of $u(x, t^n), v(x, t^n)$ respectively, and $\tau$ is the time step. To begin with, we estimate the right-hand side of the above equality in the following lemma.

**Lemma 3.4.** Denote

$$h(x) = x - \frac{\tau}{\epsilon} M(x) F'(x); \quad x \in [-\beta, \beta], \quad (3.3.8)$$

where $F'(x)$ satisfies (3.3.4). Then, we have

$$\max_{|x| \leq \beta} h(x) = h(\beta) = \beta; \quad \min_{|x| \leq \beta} h(x) = h(-\beta) = -\beta, \quad (3.3.9)$$

under the condition

$$\tau \max_{x \in [-\beta, \beta]} (M'(x)F'(x) + M(x)F''(x)) \leq \epsilon. \quad (3.3.10)$$

**Proof.** By (3.3.4), it is easy to observe that

$$h(\beta) = \beta; \quad h(-\beta) = -\beta. \quad (3.3.11)$$
It is sufficient to show that $h'(x) \geq 0$ holds in $[-\beta, \beta]$. Since

$$h'(x) = 1 - \frac{\tau}{\epsilon}(M'(x)F'(x) + M(x)F''(x)),$$  \hspace{1cm} (3.3.12)

the condition (3.3.10) is sufficient to guarantee (3.3.9). \hfill \square

We denote by $\| \cdot \|_{\infty}$ the usual infinity norm for a function or for a matrix.

**Theorem 3.5.** Assume the initial value satisfies

$$\|u_0(x)\|_{\infty} \leq \beta,$$  \hspace{1cm} (3.3.13)

and the time step size $\tau$ satisfies the condition (3.3.10). Then the scheme (3.3.6), with periodic boundary conditions, homogeneous Neumann boundary conditions or homogeneous Dirichlet boundary conditions, preserves the maximum principle, i.e.,

$$\|u^n\|_{\infty} \leq \beta, \quad \text{for all } n \geq 0.$$  \hspace{1cm} (3.3.14)

**Proof.** We proceed by induction. By assumption, the result is true for $n = 0$. Assume the result holds for $n \leq m$ i.e. $\|u^m\|_{\infty} \leq \beta$. Next we check this holds for $n = m + 1$.

By (3.3.7) and the definition of $h(x)$, we get

$$u^{m+1} + \tau \mathbf{v} \cdot \nabla u^{m+1} - \tau \epsilon M(u^m) \Delta u^{m+1} = h(u^m).$$  \hspace{1cm} (3.3.15)

By Lemma 3.4 and $\|u^m\|_{\infty} \leq \beta$, we find

$$\|h(u^m)\|_{\infty} \leq \beta \quad \text{and} \quad M(u^m) \geq 0.$$  \hspace{1cm} (3.3.16)

Assume the boundary value problem (3.3.15) achieves the maximum at $x^*$ inside $\Omega$, thus

$$\nabla u^{m+1}(x^*) = \mathbf{0}, \quad \Delta u^{m+1}(x^*) \leq 0.$$  \hspace{1cm} (3.3.17)

Hence

$$\max(u^{m+1}) \leq h(u^m(x^*)).$$  \hspace{1cm} (3.3.18)

Similarly, we can get

$$\min(u^{m+1}) \geq h(u^m(x^{**})).$$  \hspace{1cm} (3.3.19)
Since the boundary values are bounded by $\beta$, we find

$$\|u^{m+1}\|_\infty \leq \|\hat{h}(u^m)\|_\infty \leq \beta.$$  \hfill (3.3.20)

The proof is complete.

We observe that the time step constraint (3.3.10) can be very severe when $\epsilon \ll 1$. To reduce the time step restriction, we consider the stabilized scheme (cf. [43])

$$\frac{u^{n+1} - u^n}{\tau} + \mathbf{v}^{n+1} \cdot \nabla u^{n+1} + S(u^{n+1} - u^n) = M(u^n)(\epsilon \Delta u^{n+1} - \frac{1}{\epsilon} F'(u^n),$$  \hfill (3.3.21)

where $S \geq 0$ is a stabilizing parameter to be determined.

Corollary 3.1. Assume the initial value satisfies

$$\|u_0(x)\|_\infty \leq \beta, \quad (3.3.22)$$

and the time step size $\tau$ satisfies the following condition

$$\frac{1}{\tau} + S \geq \frac{1}{\epsilon \max_{x \in [-\beta, \beta]} (M'(x)F'(x) + M(x)F''(x))}. \quad (3.3.23)$$

Then the scheme (3.3.21), with periodic boundary conditions, homogeneous Neumann boundary conditions or homogeneous Dirichlet boundary conditions, preserves the maximum principle, i.e.,

$$\|u^n\|_\infty \leq \beta, \quad \text{for all } n \geq 0.$$  \hfill (3.3.24)

The proof is similar to that of Theorem 3.5, so we will omit it here. In following sub-sections, we also omit the proof for the stabilized schemes as their proof is similar to that for the non-stabilized semi-implicit schemes.

3.3.2 The fully discrete semi-implicit scheme

In this section, we construct fully discrete semi-implicit schemes with finite differences for the spatial variable. Although the proofs are also valid for periodic or
homogeneous Neumann boundary conditions, for simplicity, we assume that Ω is a rectangular domain with homogeneous Dirichlet boundary conditions.

We first consider the 1D case. We handle the diffusion term by the central finite difference method. The discrete matrix $D_h$ is the same as given in the first section. Then we handle the advection term by the upwind scheme

$$au_x = a^+ u_i^- + a^- u_i^+,$$  \hspace{1cm} (3.3.25)

where $a^+$, $a^-$ are defined as

$$a^+ = \max\{0, a\}, \quad a^- = \min\{0, a\},$$  \hspace{1cm} (3.3.26)

and $u_i^-$, $u_i^+$ are defined as

$$u_i^- = \frac{-u_{i-1} + u_i}{h}, \quad u_i^+ = \frac{u_{i+1} - u_i}{h}.$$  \hspace{1cm} (3.3.27)

Let us denote

$$\Lambda_1 = \text{diag}(\text{abs}(V^{n+1})), \quad \Lambda_2 = \text{diag}(M(U^n)),$$  \hspace{1cm} (3.3.28)

where $V$ is a vector, $\text{diag}(V)$ is the diagonal matrix with diagonal elements being components of $V$,

$$\text{abs}(V^{n+1}) = (|v_1^{n+1}|, |v_2^{n+1}|, \cdots, |v_N^{n+1}|)^T, \quad M(U^n) = (M(u_1^n), M(u_2^n), \cdots, M(u_1^n))^T,$$

and

$$A_v = \frac{1}{h} \begin{bmatrix}
-1 & \frac{1-\text{sign}(v_1^{n+1})}{2} & \cdots & \cdots & \frac{1-\text{sign}(v_N^{n+1})}{2} \\
\frac{1+\text{sign}(v_1^{n+1})}{2} & -1 & \cdots & \cdots & \frac{1-\text{sign}(v_N^{n+1})}{2} \\
\cdots & \cdots & \cdots & \cdots & \cdots \\
\frac{1+\text{sign}(v_1^{n+1})}{2} & \cdots & \cdots & -1 & \frac{1-\text{sign}(v_N^{n+1})}{2} \\
\frac{1+\text{sign}(v_1^{n+1})}{2} & \cdots & \cdots & \cdots & -1 \\
\end{bmatrix}_{N \times N}.$$  

We consider the fully discrete version of the semi-discrete scheme (3.3.7)

$$U^{n+1} - \tau \Lambda_1 A_v U^{n+1} - \tau \epsilon \Lambda_2 D_h U^{n+1} = h(U^n),$$  \hspace{1cm} (3.3.29)

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and the fully discrete version of the stabilized scheme (3.3.21)

\[ U^{n+1} + S\tau U^{n+1} - \tau \Lambda_1 A_v U^{n+1} - \tau \epsilon \Lambda_2 D_h U^{n+1} = h(U^n) + S\tau U^n. \quad (3.3.30) \]

where \( U^n \) represents the vector of numerical solution and \( h(U^n) = (h(U^n_1), h(U^n_2), \ldots, h(U^n_N))^T \), and \(-\Lambda_1 A_v\) represents the differential matrix for the advection term.

**Theorem 3.6.** Assume that \( \max_{x \in \Omega} |u_0(x)| \leq \beta \). Then,

- the fully discrete scheme (3.3.29) preserves the maximum principle in the sense that \( \|U^n\|_\infty \leq \beta \), provided that the condition (3.3.10) is satisfied;

- the stabilized fully discrete scheme (3.3.30) preserves the maximum principle in the sense that \( \|U^n\|_\infty \leq \beta \) provided that the condition (3.3.23) is satisfied.

**Proof.** We proceed by induction. Obviously, \( \|U^0\|_\infty \leq \max_{x \in \Omega} |u_0(x)| \leq \beta \). We assume the result holds for \( n \leq m \) i.e. \( \|U^m\|_\infty \leq \beta \). Next we check this holds for \( n = m + 1 \). Denote

\[ G = \tau \Lambda_1 A_v + \tau \epsilon \Lambda_2 D_h. \quad (3.3.31) \]

The linear scheme (3.3.29) becomes

\[ U^{m+1} = (I - G)^{-1} h(U^m). \quad (3.3.32) \]

By Lemma 3.4 and \( \|U^m\|_\infty \leq \beta \), we find

\[ \|h(U^m)\|_\infty \leq \beta. \quad (3.3.33) \]

Meanwhile, it easy to check \( G \) is an negative diagonally dominant matrix. Hence, due to Lemma 3.3, we have

\[ \|(I - G)^{-1}\|_\infty \leq 1. \quad (3.3.34) \]

Consequently,

\[ \|U^{m+1}\|_\infty \leq \|(I - G)^{-1}\|_\infty \|h(U^m)\|_\infty \leq \beta. \quad (3.3.35) \]

The result for the stabilized scheme (3.3.30) can be established in a similar fashion.
We also note that Hoff has studied finite difference schemes for the general reaction-diffusion system in [88], which adopted second-order central finite difference scheme in space and first-order weighted linear semi-implicit scheme in time. Unlike Hoff, we use the first-order implicit upwind scheme to handle advection term to avoid Courant-Friedrichs-Lewy condition constraint. Hence, we achieve the numerical maximum principle without any spatial mesh grid restriction.

Now we extend our attention to multi-dimensional case. For brevity, we just point out the main idea for the multi-dimensional case. We can see that the analysis in the 1-D case focuses on obtaining $L^\infty$ estimate for the solution to one linear system. We achieve it by two steps: the $L^\infty$ norm of the system matrix $I - G$ and the $L^\infty$ norm of the right-hand side $h(U^m)$. For multi-dimensional case, the estimate for the right-hand side is exactly the same as the 1-D case since we accomplish it point-wisely. If we also use central finite difference method to handle the diffusion term and upwind scheme to handle the advection term, we can still ensure the stiff matrix negative diagonally dominant. So $L^\infty$ norm of the stiff matrix for the multi-dimensional case can be bounded in the same way as in the 1-D case. In summary, the conditions to guarantee the maximum principle do not change are the same as in the 1-D case.

3.3.3 Logarithmic free energy with nonlinear degenerate mobility

The results in the last two sections were derived with the general assumptions (3.3.3)-(3.3.4) for the potential function $F(u)$ and (3.3.5) for the mobility function $M(u)$. In this section, we apply the previous results to two cases commonly used in practice. The first example is the Allen-Cahn equation in its simplest form: the mobility $M(u) = 1$ and

$$F(u) = \frac{1}{4}(u^2 - 1)^2, \quad F'(u) = u^3 - u.$$  \hspace{1cm} (3.3.36)
In this case, we find the same result in the previous section. We now consider a more complicated situation with a logarithmic free energy function

$$
F(u) = \frac{\theta}{2}[(1 + u) \ln(1 + u) + (1 - u) \ln(1 - u)] - \frac{\theta_c}{2} u^2, \quad (3.3.37)
$$

where $\theta < \theta_c$ are two positive constants, and a degenerated nonlinear mobility

$$
M(u) = D(1 - u^2), \quad (3.3.38)
$$

which more accurately describe the physics of phase separation, as pure phases must have vanishing mobility. Numerical analysis on Cahn-Hilliard equations can be found in [91, 92] and references therein.

In this case, we have

$$
F'(u) = \frac{\theta}{2} \ln \left( \frac{1 + u}{1 - u} \right) - \theta_c u. \quad (3.3.39)
$$

We derive from (3.3.39) that $\beta$ is the positive root of

$$
\frac{1}{2\beta} \ln \frac{1 + \beta}{1 - \beta} = \frac{\theta_c}{\theta} \quad (3.3.40)
$$

Hence, the extreme points $\pm \alpha$ of $F'(u)$ are given by

$$
\alpha = \sqrt{1 - \frac{\theta}{\theta_c}} = \sqrt{1 - \frac{2\beta}{\ln \frac{1 + \beta}{1 - \beta}}}. \quad (3.3.41)
$$

It is not difficult to show that

$$
1 - \beta^2 < \frac{2\beta}{\ln \frac{1 + \beta}{1 - \beta}}, \quad \forall \beta \in (0, 1). \quad (3.3.42)
$$

Consequently, we have $\alpha < \beta$. A sketch of $f(x)$ is presented in Fig. 3.5.

For this case, we have the following result:

**Corollary 3.2.** Assume $\max_{x \in \Omega} |u_0(x)| \leq \beta$. Then the fully discrete scheme (3.3.29) with (3.3.37)-(3.3.38) preserves the maximum principle in the sense that $\|U^n\|_\infty \leq \beta$ provided that

$$
0 < \tau \leq \frac{\epsilon}{D(\theta - (1 - 3\beta^2)\theta_c)}; \quad (3.3.43)
$$
and the stabilized fully discrete scheme (3.3.30) with (3.3.37)-(3.3.38) preserves the maximum principle in the sense that \( \|U^n\|_\infty \leq \beta \) provided

\[
\frac{1}{\tau} + S \geq \frac{D(\theta - (1 - 3\beta^2)\theta_c)}{\epsilon}.
\] (3.3.44)

**Proof.** Since

\[
M'(u) = -2Du, \quad F''(u) = \frac{\theta}{1 - u^2} - \theta_c,
\] (3.3.45)

the condition (3.3.10) is equivalent to

\[
\tau \max_{u \in [-\beta, \beta]} (\theta - \theta_c + 3\theta_c u^2 - 2\theta_c u \ln \frac{1 + u}{1 - u}) \leq \frac{\epsilon}{D}.
\] (3.3.46)

It is nontrivial and not necessary to get the analytical maximum value in the above inequality, so we just offer a sufficient condition here.

One observes that \( u \ln \frac{1 + u}{1 - u} \geq 0 \) holds in \([-\beta, \beta]\). Hence, a sufficient condition for (3.3.46) is

\[
\tau \max_{u \in [-\beta, \beta]} (\theta - \theta_c + 3\theta_c u^2) \leq \frac{\epsilon}{D}.
\] (3.3.47)

Furthermore, by (3.3.40) and (3.3.42), we have

\[
\theta > (1 - \beta^2)\theta_c.
\] (3.3.48)

Combining the above two inequalities yields the desired result (3.3.43). The other case can be proved similarly.
3.3.4 Error analysis

While it is relatively easy to establish some stability results for numerical schemes to the Allen-Cahn type equations, it is non-trivial to derive their error estimates in the case with nonlinear degenerated mobility. The main difficulty for deriving such estimates is the lack of discrete maximum principle, so that the nonlinear degenerated mobility can become negative. With the results we established in previous sections, we are now in position to establish error estimates for the fully discrete semi-implicit schemes.

We consider first the scheme (3.3.29), which can be concisely rewritten as

\[
(I - \tau \Lambda_1 A_v - \tau \epsilon \Lambda_2 (U^{n-1})) U^n = U^{n-1} - \frac{\tau}{\epsilon} \Lambda_2 (U^{n-1}) F'(U^{n-1}),
\]

where \( \Lambda_1 \) and \( \Lambda_2 \) are defined by (3.3.28). The error \( U^n \) is defined as

\[
E^n = U(t_n) - U^n,
\]

where \( U(t_n) \) is the vector consisting of values of the exact solution of (3.3.1)-(3.3.2) at the grid points.

First, we define the local truncation error \( T^n \) for the scheme (3.3.30) by

\[
T^n = (I - \tau \Lambda_1 A_v - \tau \epsilon \Lambda_2 (U(t_{n-1}))) U(t_n) - (U(t_{n-1}) - \frac{\tau}{\epsilon} \Lambda_2 (U(t_{n-1})) F'(U(t_{n-1})).
\]

We assume that the exact solution \( U(t) \) is sufficient smooth. Then, it is easy to show that

\[
\|T^j\|_\infty \leq c \tau \eta \quad \text{for} \quad j \leq n,
\]

where \( \eta = \tau + h \) and \( c = c(t_n) \) is a positive function of \( t_n \) which may depend on \( U(t) \) but not on \( \tau \) or \( h \). Denote

\[
S^N_\beta = \{ x \in \mathbb{R}^N : \|x\|_\infty \leq \beta \}.
\]

Then with the assumptions (3.3.3)-(3.3.4) and (3.3.5), we have \( U^n, U(t_n) \in S^N_\beta \).
We assume that there exist \( \kappa_i > 0 \) \((i = 1, 2, 3, 4)\) such that for any \( p, q \in S^N_\beta \), we have

\[ \|
\Lambda_2(p) - \Lambda_2(q)\|_\infty \leq \kappa_1 \| p - q \|_\infty, \quad \| F'(p) - F'(q) \|_\infty \leq \kappa_2 \| p - q \|_\infty \]  

(3.3.54)

and

\[ \|
\Lambda_2(p)\|_\infty \leq \kappa_3, \quad \| F'(p)\|_\infty \leq \kappa_4. \]  

(3.3.55)

It is easy to see that in case of polynomial free energy, i.e., with \( M(u) = 1 \) and \( F(u) = \frac{1}{4}(u^2 - 1)^2 \), we can choose \( \kappa_1 = 1, \kappa_2 = 2, \kappa_3 = 1 \) and \( \kappa_4 = \frac{2}{3\sqrt{3}} \). In the case with \( F(u) \) and \( M(u) \) given by (3.3.37) and (3.3.38), we can take \( \kappa_1 = 2\beta D, \kappa_2 = \frac{\theta}{1-\beta^2} - \theta_c, \kappa_3 = D \) and \( \kappa_4 = F'(-\alpha) \) where \( \alpha, \beta \) and \( D \) are given in (3.3.41), (3.3.40) and (3.3.38), respectively. We emphasize that these constants are all independent of the mesh size in both cases.

**Theorem 3.7.** Assume that the solution \( u(x, t) \) of (3.3.1)-(3.3.2) is sufficiently smooth and \( \max_{x \in \Omega} |u_0(x)| \leq \beta \). Then, we have the following error estimate for the scheme (3.3.49):

\[ \| E^n \|_\infty \leq e^\epsilon t_n (\| E^0 \|_\infty + c t_n (\tau + h)) \]  

(3.3.56)

with

\[ \kappa = \epsilon \beta \kappa_1 + \frac{\kappa_1 \kappa_4 + \kappa_2 \kappa_3}{\epsilon}, \]  

(3.3.57)

provided that \( \tau \) satisfies (3.3.10).

**Proof.** Subtracting (3.3.49) from (3.3.51), we obtain

\[ (I - \tau \Lambda_1 A_v - \tau \epsilon \Lambda_2(U^{n-1})) E^n = E^{n-1} - \tau \epsilon (\Lambda_2(U^{n-1}) - \Lambda_2(U(t_{n-1}))) U(t_{n-1}) \]

\[ - \frac{1}{\epsilon} (\Lambda_2(U(t_{n-1})) F'(U(t_{n-1})) - \Lambda_2(U^{n-1}) F'(U^{n-1})) \]

\[ + T^n = E^{n-1} + S^n_I + S^n_H + T^n. \]  

(3.3.58)

Hence

\[ E^n = (I - G)^{-1}(E^{n-1} + S^n_I + S^n_H + T^n), \]  

(3.3.59)
where $G$ is defined in (3.3.31). By (3.3.34) and (3.3.52), we have

$$
\|E^n\|_\infty \leq \|E^{n-1}\|_\infty + \|S_I\|_\infty + \|S_H\|_\infty + c\tau \eta. \quad (3.3.60)
$$

From (3.3.54) and (3.3.55), we can derive

$$
\|S^n_I\|_\infty \leq \tau \epsilon \beta_1 \|E^{n-1}\|_\infty, \quad (3.3.61)
$$

and

$$
\|S^n_H\|_\infty = \frac{1}{\epsilon} \|((\Lambda_2(U^{n-1}) - \Lambda_2(U(t_{n-1})))F(U^{n-1}) + \Lambda_2(U(t_{n-1}))) (F'(U^{n-1}) - F'(U(t_{n-1})))\|_\infty \leq \tau \frac{\kappa_4 \kappa_3 + \kappa_2 \kappa_3}{\epsilon} \|E^{n-1}\|_\infty. \quad (3.3.62)
$$

Combining (3.3.61) and (3.3.62), we find from (3.3.60) that

$$
\|E^n\|_\infty \leq (1 + \kappa \tau)\|E^{n-1}\|_\infty + c\tau \eta, \quad (3.3.63)
$$

where $\kappa$ is defined as (3.3.57). It follows by induction that

$$
\|E^n\|_\infty \leq (1 + \kappa \tau)^n \|E^0\|_\infty + c\tau \eta \sum_{j=0}^{n-1} (1 + \kappa \tau)^j \leq e^{\kappa \tau n} (\|E^0\|_\infty + c\tau \eta), \quad (3.3.64)
$$

which is the desired result (3.3.56).

Next, we will study the error estimate for the stabilized version of scheme (3.3.49) as

$$
((1 + S\tau)I - \tau \Lambda_1 A_v - \tau \epsilon \Lambda_2(U^{n-1})) U^n = (1 + S\tau) U^{n-1} - \frac{\tau}{\epsilon} \Lambda_2(U^{n-1}) F'(U^{n-1}). \quad (3.3.65)
$$

Similarly, we define the truncation error for the above scheme as

$$
T^n_S = ((1 + S\tau)I - \tau \Lambda_1 A_v - \tau \epsilon \Lambda_2(U(t_{n-1}))) U(t_n) - ((1 + S\tau) U(t_{n-1}) - \frac{\tau}{\epsilon} \Lambda_2(U(t_{n-1})) F'(U(t_{n-1}))). \quad (3.3.66)
$$
Under the similar consistency assumption as (3.3.52) for the same truncation error (3.3.51) as following
\[ \|T_j\|_\infty \leq c_3 \tau \eta \quad \text{for} \quad j \leq n, \] (3.3.67)
and the same definitions of parameters \( \kappa_1, \kappa_2, \kappa_3 \) and \( \kappa_4 \) in (3.3.54) and (3.3.55) respectively, we have the error estimate for the stabilized scheme

**Corollary 3.3.** Assume that the solution \( u(x,t) \) of (3.3.1)-(3.3.2) is sufficiently smooth and \( \max_{x \in \Omega} |u_0(x)| \leq \beta \). Then, we have the same error estimate for the scheme (3.3.65):
\[ \|E^n\|_\infty \leq e^{\kappa t_n} (\|E^0\|_\infty + c_3 t_n (\tau + h)) \] (3.3.68)
with same \( \kappa \) defined by (3.3.57) provided that \( \tau \) satisfies (3.3.23).

### 3.3.5 Numerical tests

In this section, we present some numerical experiments to verify theoretical results obtained in the previous sections.

**Example 3.2.** First, we consider the one-dimensional Allen-Cahn equation with logarithmic free energy (3.3.37) and nonlinear mobility (3.3.38) subjected to the homogeneous Dirichlet boundary condition with following initial value
\[ u_0(x) = -0.9 \sin(50x). \] (3.3.69)

The velocity field is given as
\[ v(x,t) = e^t \sin(x). \] (3.3.70)

We take the parameters \( \epsilon = 0.01, D = 1 \) and the computation domain to be \([0, 2\pi]\).

We use an equidistant mesh with \( N = 200 \) intervals, and set \( \beta = 0.94 \). Note that \( u_0(x) \) takes the value \(-0.9\) and \(0.9\) at nodes alternately. Numerical results with different time step \( \tau \) and stabilized parameter \( S \) are presented in Figs. 3.6.

We denote the constants in (3.3.43) and (3.3.44) by
\[ M_{tol} = \frac{D(\theta - (1 - 3\beta^2)\theta_c)}{\epsilon}, \quad t_{tol} = \frac{\epsilon}{D(\theta - (1 - 3\beta^2)\theta_c)}. \] (3.3.71)
For this example, we have $t_{\text{tol}} = 0.046$. First, we set stabilized parameter $S = 0$, i.e., we use the standard implicit-explicit scheme (3.3.29). The maximum of numerical solutions at different time are shown in the left part of Fig. 3.6. We can observe that when $\tau = t_{\text{tol}}$ and $\tau = 2.5t_{\text{tol}}$ the discrete maximum principle can be preserved. But if the time step $\tau = 5t_{\text{tol}}$, values greater than $\beta$ will occur. These results illustrate that (3.3.43) in Corollary 3.2 offers a sufficient but not a necessary condition to ensure the maximum principle. Then, we set $S = 0.1M_{\text{tol}}$ and plot the results in the right part of Fig. 3.6. This time, we see that the scheme preserves the discrete maximum principle even when time step $\tau = 10t_{\text{tol}}$. However, in unpresented results, the standard scheme will blow up very soon with this time step. Hence, the stabilized scheme (3.3.30) allows much larger time steps which can reduce the computational time significantly for long time simulations.

Figure 3.6: Maximum values for the case $S = 0$ (left) and $S = 0.1M_{\text{tol}}$ (right) with different time steps $\tau = t_{\text{tol}}$, $2.5t_{\text{tol}}$, $5t_{\text{tol}}$.

**Example 3.3.** In this example, we consider the 2D Allen-Cahn equation with logarithmic free energy (3.3.37) and nonlinear mobility (3.3.38) subjected to the homogeneous Dirichlet boundary condition with the following random initial value

$$u_0(x, y) = 0.05(2 \text{rand} - 1),$$  

(3.3.72)

where ‘rand’ means a random number in $[0, 1]$. And we take the clockwise rotational
velocity field $\mathbf{u}(x, y, t) = (v_1(x, y, t), v_2(x, y, t))^T$ with

$$v_1(x, y, t) = y - \pi, \quad v_2(x, y, t) = \pi - x. \quad (3.3.73)$$

We take the parameters $\epsilon = 0.1$, $D = 1$ and the computation domain to be $[0, 2\pi] \times [0, 2\pi]$. The mesh in space is fixed with $N_x = N_y = 100$, and we set $\beta = 0.95$. Then we see $t_{tot} = 0.045$. In this example, we take $S = 0$ and time step $\tau = 0.04$ which is smaller than $t_{tot}$. Evolutions and maximum values of numerical solutions are presented in Fig. 3.7. We observe in the last sub-figure that the discrete maximum principle are indeed well preserved. We also observe the ordering and coarsening phenomena as well as the rotation effect due to the advection term with a given rotational velocity field.

![Figure 3.7: Evolutions and maximum values of numerical solutions.](image)
Example 3.4. In this example, we aim to emphasize the significant function of the stabilized scheme in the long time simulations, especially equipped with time-stepping adaptivity schemes, where large time step can be safely used in the stabilized scheme considering the stability. To implement our numerical experiments efficiently, we consider the the 2D Allen-Cahn equation in $[0, 2\pi] \times [0, 2\pi]$ with logarithmic free energy (3.3.37) and constant mobility $D$ subjected to the periodic boundary condition, i.e.

$$\frac{\partial u}{\partial t} = D (\epsilon \Delta u - \frac{1}{\epsilon} F'(u)).$$

(3.3.74)

The initial value is also taken as the following random initial value

$$u_0(x, y) = 0.05(2 \text{rand} - 1).$$

(3.3.75)

We discretize the Laplace Operator by the central finite difference. Due to the periodic boundary condition, fast solvers can be applied.

We take the parameters $\epsilon = 0.04$ and $D = 2$. Same as in Example 3.3, the mesh in space is fixed with $N_x = N_y = 100$, and we set $\beta = 0.95$. In this case, the time step size constraint (3.3.23) is equivalent to

$$\frac{1}{\tau} + S \geq \frac{D}{\epsilon} \left( \frac{\theta}{1 - \beta^2} - \theta_c \right) =: M_{tol}.$$  

(3.3.76)

The standard scheme require time step smaller than $t_{tol} = \frac{1}{M_{tol}} = 0.0046$.

First, we obtain the reference solution by the standard scheme with very small uniform time step as $\tau = 0.0001$, which is shown in Fig. 3.8. Then we implement the stabilized scheme by following the main idea of the adaptive time-stepping algorithm given in [41]. We update the time step using the equation

$$A_{\phi}(\epsilon, \tau) = \rho \left( \frac{tol}{\epsilon} \right)^{1/2}. $$

(3.3.77)

Our default values for the safety coefficient $\rho$ and the tolerance $tol$ are taken same as in [41], i.e., $\rho = 0.9$ and $tol = 10^{-3}$. The maximum time step $\tau_{max}$ allowed during simulations is taken as 0.01. We set the initial time step same as one used in reference solutions 0.0001 and initial stabilized parameter $S = 0$. 

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Figure 3.8: Evolutions and maximum values of numerical solutions obtained by standard scheme with constant time step $\tau = 0.0001$.

Note that the stabilized parameter is also adaptive in our algorithm. The reason is natural. Since $S \geq M_{\text{tol}} - \frac{1}{\tau}$ is a sufficient condition to guarantee the numerical maximum principle. This stability requirement seems more important in the logarithmic free energy case, because complex values in solutions will produce soon once we get solutions against the maximum principle. On the other hand, we also observe that effective time step will be obviously smaller than the time step used in the stabilized
Algorithm 1 Time step and stabilized coefficient adaptive procedure

Given: $U^n$, $\tau_n$ and stabilized parameter $S_n$.

Step 1. Compute $U_{FE}^{n+1}$ by the Forward Euler method with $\tau_n$.

Step 2. Compute $U^{n+1}$ by the stabilized scheme method with $\tau_n$ and $S_n$.

Step 3. Calculate $e_{n+1} = \frac{||U_{FE}^{n+1} - U^{n+1}||}{||U^{n+1}||}$

Step 4. if $e_{n+1} > tol$, then

Recalculate time step $\tau_n \leftarrow \min\{A_p(e_{n+1}, \tau_n), \tau_{max}\}$ and
stabilized parameter $S_n \leftarrow \min\{0, M_{tol} - \frac{1}{\tau_n}\}$

Step 5. goto Step 1

Step 6. else

Update time step $\tau_{n+1} \leftarrow \min\{A_p(e_{n+1}, \tau_n), \tau_{max}\}$ and
stabilized parameter $S_{n+1} \leftarrow \min\{0, M_{tol} - \frac{1}{\tau_{n+1}}\}$

Step 7. endif

Evolutions and maximum values of numerical solutions are shown in Fig. 3.9, and the adaptive time steps and stabilized parameters are shown in Fig. 3.10. Comparing the numerical result in Fig. 3.9 with reference solutions, we observe that evolutions coincide quite well with the reference one with very smaller time step, especially before $T = 5$. In the left of Fig. 3.10, we can see the efficiency is enhanced significantly, since the time step used in the adaptive algorithm is much larger one used in reference solutions. We also observe that there is some small difference in the last evolution. This can be explained in right of Fig. 3.10, in which we can see the stabilized parameters increase very soon at about $T = 9$ where the time step is taken $\tau_{max}$. Due to large stabilized parameters used, the effective time step is smaller than the time step used in the stabilized scheme, then the lagging effect is caused. Hence, we should take balance between the efficiency and accuracy in the practical simulations. But our stabilized scheme equipped with adaptive algorithms can offer an efficient
Figure 3.9: Evolutions and maximum values of numerical solutions obtained by stabilized scheme with adaptive time-stepping algorithm.
and stable tool to simulate this kind of phase-field equations in long time.

Figure 3.10: Adaptive time stepsize and adaptive stabilized parameters.

3.4 Discrete maximum principle for the fractional-in-space Allen-Cahn equation

3.4.1 Introduction

In this section, we study the numerical maximum principle of the fractional-in-space Allen-Cahn equation (FiSAC)

\[
\frac{\partial u}{\partial t} = -\epsilon^2 (-\Delta)^{\alpha/2} u - f(u), \quad x \in \Omega, \ t \in (0, T],
\]

\[
u(x, 0) = u_0(x), \quad x \in \bar{\Omega},
\]

\[
u|_{\partial \Omega} = 0,
\]

where \(\Omega\) is a bounded regular domain in \(R^d\) (\(d = 1, 2, 3\)), \(\alpha \in (1, 2)\), and the nonlinear source term is taken as the same as in the standard Allen-Cahn equation. The fractional Laplacian operator is defined same as the first section.

Fractional models, in which a standard time or space differential operator is replaced by a corresponding fractional differential operator, have a long history in, for example, physics, finance and hydrology, with such models often being used to represent so-called anomalous diffusion. As the analytical solutions can not be obtained, there have been increasing efforts in studying numerical methods for solving
the fractional differential equations. For the time fractional problems, finite difference schemes and spectral methods have been investigated, see, e.g., [69, 70, 71, 73].

In recent years, there has been tremendous interest in using the diffusive-interface phase-field approach for modeling the mesoscale morphological pattern formation and interface motion. It is noted that the combination of the fractional model and the Allen-Cahn model, namely, the fractional-in-space Allen-Cahn equation (3.4.1), is a challenging mathematical and numerical problem. It has attracted attentions in recent years. For problem (3.4.1), Burrage et al. [67] proposed an efficient implicit finite element scheme, Bueno-Orovio et al. [72] considered the Fourier spectral methods. Zhuang et al. [74] considered the finite difference method for fractional-in-space reaction diffusion equation with a nonlinear source term that satisfies the Lipschitz condition.

In the previous sections, we establish the numerical maximum principle for non-fractional Allen-Cahn equations. In this section, we wish to see if this maximum principle still holds for the numerical solutions of the FiSAC equation (3.4.1). To this end, we consider a couple of standard fully discretized schemes for (3.4.1), i.e., we use the first-order implicit-explicit scheme or second-order Crank-Nicolson scheme in time and the second-order finite difference approximation in space. The main targets are of two folds. First, we will prove that the numerical solutions will satisfy the maximum principle in the sense mentioned above. Secondly, we will show that the discrete energy of the numerical solutions decay with time.

We close this section by describing our numerical scheme for solving the FiSAC problem (3.4.1)-(3.4.3). This is done by using the finite difference method described in the first section together with the standard first-order implicit-explicit (linear) scheme or the second-order Crank-Nicolson (nonlinear) scheme in time. More precisely, we have

$$\frac{U^{n+1} - U^n}{\tau} + ((U^n)^3 - U^n) = \epsilon^2 D_h U^{n+1}$$ (3.4.4)
and
\[
\frac{U^{n+1} - U^n}{\tau} + \frac{(U^{n+1})^3 - U^{n+1}}{2} + \frac{(U^n)^3 - U^n}{2} = \frac{c^2(D_h(U^{n+1}) + D_hU^n)}{2},
\]
(3.4.5)
where \(\tau\) denotes the time stepsize, \(U^n\) represents the vector of numerical solution, and
\[
(U^n)^3 := ((U^n_1)^3, (U^n_2)^3, \cdots, (U^n_N)^3)^T.
\]
In the sense of the truncation error, the approximation (3.4.4) is of order \(O(\tau + h^2)\) and (3.4.5) is of order \(O(\tau^2 + h^2)\).

### 3.4.2 The discrete maximum principle

**Theorem 3.8.** Assume the initial value satisfies \(\max_{x \in \Omega} |u_0(x)| \leq 1\). Then the fully discrete scheme (3.4.4) preserves the maximum principle in the sense that \(\|U^n\|_\infty \leq 1\) for all \(n \geq 1\) provided that the time stepsize satisfies \(0 < \tau \leq \frac{1}{2}\).

The basic idea is quite similar to that used in Theorem 3.1.

**Theorem 3.9.** Assume the initial value satisfies \(\max_{x \in \Omega} |u_0(x)| \leq 1\). Then the fully discrete scheme (3.4.5) preserves the maximum principle in the sense that \(\|U^n\|_\infty \leq 1\) for all \(n \geq 1\) provided that the time stepsize satisfies
\[
0 < \tau \leq \min \left\{ \frac{1}{2}, \frac{h^a}{2de^2} \right\},
\]
(3.4.6)
where \(d\) is the dimension number.

**Proof.** Again we will prove this theorem by induction. It follows from the scheme (3.4.5) that
\[
\left(1 - \frac{\tau}{2}\right) U^{m+1} + \frac{\tau}{2}(U^{m+1})^3 - \frac{\tau c^2}{2}D_hU^{m+1} = \left(I + \frac{\tau c^2}{2}D_h\right)U^m + \frac{\tau}{2}(U^m - (U^m)^3).
\]
(3.4.7)
By Lemma 3.2, we have
\[
\left\| \left(1 - \frac{\tau}{2}\right) U^{m+1} + \frac{\tau}{2}(U^{m+1})^3 - \frac{\tau c^2}{2}D_hU^{m+1} \right\|_\infty \geq \left(1 - \frac{\tau}{2}\right) \|U^{m+1}\|_\infty + \frac{\tau}{2} \|U^m - (U^m)^3\|_\infty.
\]
(3.4.8)
Let $H = \frac{1}{2} I + \frac{\tau^2}{2} D_h$. Then
\[
\left( I + \frac{\tau^2}{2} D_h \right) U^m + \frac{\tau}{2} (U^m - (U^m)^3) = H U^m + \frac{U^m + \tau (U^m - (U^m)^3)}{2}.
\]

(3.4.9)

It is easy to verify that the matrix $H = (h_{ij})$ in the $d$-dimension satisfies
\[
i) h_{ii} = \frac{1}{2} - \frac{d \tau c^2 (\alpha^2 + \alpha - 2)}{4 h^a (- \cos \frac{\pi}{2} \alpha)}, \quad ii) h_{ij} | j \neq i \geq 0 \quad \text{and} \quad \max_i \sum_j h_{ij} \leq \frac{1}{2}.
\]

(3.4.10)

If we assume $h_{ii} \geq 0$, i.e.,
\[
\tau \leq \frac{2 h^a (- \cos \frac{\pi}{2} \alpha)}{dc^2 (\alpha^2 + \alpha - 2)},
\]
then $H$ is non-negative, i.e., $h_{ij} \geq 0$ for $1 \leq i, j \leq N$. Consequently,
\[
\|H\|_\infty = \max_i \sum_j |h_{ij}| = \max_i \sum_j h_{ij} \leq \frac{1}{2}.
\]

(3.4.12)

We further denote
\[
p(\alpha) := \frac{- \cos \frac{\pi}{2} \alpha}{\alpha^2 + \alpha - 2}.
\]

(3.4.13)

It is easy to verify that
\[
\frac{1}{4} < p(\alpha) < \frac{\pi}{6}, \quad \text{for} \quad \alpha \in (1, 2).
\]

(3.4.14)

This allows us to simplify the constraint imposed on time step (3.4.11) as
\[
\tau \leq \frac{h^a}{2 dc^2}.
\]

(3.4.15)

Now consider the last term of (3.4.9). If $\|U^m\|_\infty \leq 1$, using the argument for $g(x)$ in the proof of Theorem 3.8 gives
\[
\|U^m + \tau (U^m - (U^m)^3)\|_\infty \leq 1, \quad 0 < \tau \leq \frac{1}{2}.
\]

(3.4.16)

If $\|U^m\|_\infty \leq 1$, then combining (3.4.12) and (3.4.16) yields
\[
\left\| \left( I + \frac{\tau^2}{2} D_h \right) U^m + \frac{\tau}{2} (U^m - (U^m)^3) \right\|_\infty
\leq \|H\|_\infty \|U^m\|_\infty + \frac{1}{2} \|U^m + \tau (U^m - (U^m)^3)\|_\infty \leq \frac{1}{2} + \frac{1}{2} = 1,
\]

(3.4.17)
provided that the condition (3.4.6) is satisfied. Consequently, using (3.4.8) gives

$$\left(1 - \frac{\tau}{2}\right)\|U^{m+1}\|_\infty + \frac{\tau}{2}\|U^{m+1}\|_\infty^3 \leq 1,$$

(3.4.18)

which yields \(\|U^{m+1}\|_\infty \leq 1\). This completes the proof. \(\square\)

### 3.4.3 The discrete energy stability

After being semi-discretized in space, an ODE system is obtained

$$\frac{dU}{dt} = \epsilon^2 D_h U + U - U^3,$$

(3.4.19)

where \(D_h\) is given by (3.1.9)-(3.1.11) for one to three space dimensions, respectively. If we define the following discrete energy:

$$E_h(U) = \frac{1}{4} \sum_{i=1}^{N} (U_i^2 - 1)^2 - \frac{\epsilon^2}{2} U^T D_h U,$$

(3.4.20)

then the ODE system (3.4.19) can be viewed as the gradient flow of the energy \(E_h(U)\), i.e.,

$$\frac{dU}{dt} = -\nabla_U E_h(U).$$

(3.4.21)

Taking \(L^2\) inner product of (3.4.21) with \(-\frac{dU}{dt}\) yields

$$\frac{dE_h(U)}{dt} = -\left\|\frac{dU}{dt}\right\|_2^2 \leq 0,$$

(3.4.22)

which implies that the energy \(E_h(U)\) defined by (3.4.20) decays with time. Our next task is to show that this energy stability can be inherited by both the first-order scheme (3.4.4) and the second-order scheme (3.4.5).

**Theorem 3.10.** Under the conditions in Theorem 3.8, the numerical solutions obtained by the scheme (3.4.4) can guarantee the discrete energy decay properly, i.e.,

$$E_h(U^{n+1}) \leq E_h(U^n), \text{ for } n = 0, 1, 2, \cdots$$

(3.4.23)

The proof is similar to Theorem 3.2, so we skip it here.
Theorem 3.11. Under the conditions in Theorem 3.9, the numerical solutions obtained by the scheme (3.4.5) can guarantee the discrete energy decay properly, i.e.,

\[ E_h(U^{n+1}) \leq E_h(U^n), \text{ for } n = 0, 1, 2, \cdots. \] (3.4.24)

Proof. First, we take the difference of the discrete energy between two time level

\[ E_h(U^{n+1}) - E_h(U^n) \] (3.4.25)

\[ = \frac{1}{4} \sum_{i=1}^{N} \left[ ((U_i^{n+1})^2 - 1)^2 - ((U_i^n)^2 - 1)^2 \right] - \frac{\epsilon^2}{2} \left( (U_i^{n+1})^T D_h U^{n+1} - (U_i^n)^T D_h U^n \right). \]

Taking \( L^2 \) inner product of (3.4.5) with \((U_i^{n+1} - U_i^n)^T\) obtains

\[ \frac{\epsilon^2}{2} (U_i^{n+1} - U_i^n)^T D_h (U_i^{n+1} + U_i^n). \] (3.4.26)

Since the discrete Laplace operator \( D_h \) is symmetric, we have

\[ \frac{\epsilon^2}{2} (U_i^{n+1} - U_i^n)^T D_h (U_i^{n+1} + U_i^n) = \frac{\epsilon^2}{2} \left( (U_i^{n+1})^T D_h U^{n+1} - (U_i^n)^T D_h U^n \right). \] (3.4.27)

Note that for any \( a, b \in \mathbb{R} \)

\[ (a^3 - a)(a - b) + (a - b)^2 \geq \frac{1}{4} \left[ (a^2 - 1)^2 - (b^2 - 1)^2 \right]. \] (3.4.28)

Under the conditions in Theorem 3.9, we have \( \|U^{n+1}\|_\infty \leq 1 \) and \( \|U^n\|_\infty \leq 1 \). Consequently, it follows from (3.2.12) and (3.4.28) that

\[ \frac{1}{4} \sum_{i=1}^{N} \left[ ((U_i^{n+1})^2 - 1)^2 - ((U_i^n)^2 - 1)^2 \right] \] (3.4.29)

\[ \leq \sum_{i=1}^{N} \left[ \frac{1}{2} ((U_i^{n+1})^3 - U_i^{n+1})(U_i^{n+1} - U_i^n) + \frac{1}{2} ((U_i^n)^3 - U_i^n)(U_i^{n+1} - U_i^n) + (U_i^{n+1} - U_i^n)^2 \right]. \]

This together with (3.4.25) and (3.4.26)-(3.4.27), yield

\[ E_h(U^{n+1}) - E_h(U^n) \leq \left( 1 - \frac{1}{\tau} \right) \sum_{i=1}^{N} (U_i^{n+1} - U_i^n)^2. \] (3.4.30)
Since $0 < \tau \leq \frac{1}{2}$, the right-hand side of (3.4.30) is non-positive,\
\[ E_h(U^{n+1}) - E_h(U^n) \leq 0, \]  
(3.4.31)
which implies that (3.4.24) holds. \hfill \square

We close this section by pointing out that although the above energy stability result for the Crank-Nicolson scheme is conditional, our numerical experiments show that the condition (3.4.6) may be removed, i.e., the energy stability may be unconditional. It is noted Qiao et al. [58] obtained an unconditional energy stability result for the modified Crank-Nicolson approximation for a relevant phase-field model.

3.4.4 Numerical examples

In this sub-section, we present a number of numerical experiments to verify the theoretical results obtained in the previous sections. We consider the one-dimensional FiSAC equation in the first two examples and two-dimensional problem in the third example.

Example 3.5. This example uses the first order scheme (3.4.4) with the initial value

\[ u_0(x) = \begin{cases} 
\frac{\sqrt{3}}{2} - 200\sqrt{3}(x - 0.05)^2, & 0 \leq x \leq 0.05, \\
\frac{\sqrt{3}}{2}, & 0.05 < x < 0.95, \\
\frac{\sqrt{3}}{2} - 200\sqrt{3}(x - 0.95)^2, & 0.95 \leq x \leq 1.
\end{cases} \]

The mesh size in space is fixed as $h = 0.01$, and the time step $\tau$ and the fractional derivative parameter $\alpha$ are varied. For the first-order implicit-explicit scheme (3.4.4) with $\alpha = 1.5$ and the parameter $\epsilon = 0.01$, it can be observed from Fig. 3.11 that the discrete maximum principle is preserved for $\tau = 0.5$. However, the maximum value exceeds 1 for $\tau > 0.5$, such as $\tau = 1$ and 1.5. This result is consistent with the theoretical prediction of Theorem 3.8. With the same parameters setting, we plot the energy curve and observe that the energy decay property does not hold for $\tau > 0.5$. This result is consistent with the prediction of Theorem 3.10.
Figure 3.11: Example 3.5 with scheme (3.4.4): (a) the maximum values with different times steps ($\alpha = 1.5$, $\epsilon = 0.01$); (b) energy curve with different times steps ($\alpha = 1.5$, $\epsilon = 0.01$).

In Fig. 3.12, we choose $\tau = 0.01$ and $\epsilon = 0.2$ and plot the numerical solutions at $t = 20$ with different fractional parameters $\alpha$. It is observed that the numerical solutions become more gentle when $\alpha$ varies from 2 to 1.1.

**Example 3.6.** The second example is concerned with the second-order scheme (??) with $\alpha = 1.5$. The following initial condition is used

$$u_0(x) = 0.95 \times \text{rand}(\cdot) + 0.05,$$

where $\text{rand}(\cdot)$ represents a random number on each point in $(0, 1)$, and zero boundary values are set for $u_0(x)$.  

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We fix the mesh size in space as $h = 0.1$ and the nonlinear equation (3.4.5) is solved by Newton’s iteration method which turns out to be very efficient. Note the initial guess at each Newton iteration is obtained by using the linear scheme (3.4.4). It is observed that the maximum principle is indeed decided by the condition (3.4.6).

To explain this more clearly, we denote $\theta = \frac{h^\alpha}{2\epsilon_2}$. For the case $\epsilon = 0.1$ (recall $h = 0.1$), we have $\theta \approx 1.581$, which implies that the condition (3.4.6) becomes $\tau \leq 0.5$. In the top two sub-figures of Fig. 3.13, the maximum value of numerical solution is bounded by 1 for $\tau = 0.4$ and exceeds 1 if $\tau = 1.5$. If we change $\epsilon$ to be 0.9, then we obtain $\theta \approx 0.0195$, which implies that the condition (3.4.6) becomes $\tau \leq 0.0195$. Indeed we observe that the maximum value is preserved if $\tau = 0.01$ and is not preserved if $\tau = 0.4$.

**Example 3.7.** Consider the first order scheme (3.4.4) with following initial value in two-space dimension:

$$u_0(x, y) = 0.1 \times \text{rand}(\cdot) - 0.05,$$

where rand(\cdot) represents a random number on each point in $(0, 1)^2$. Zero boundary value is set for $u_0(x, y)$.

We fix $\alpha = 1.5$, $\epsilon = 0.02$ and $h_x = h_y = 0.01$, while the time step $\tau$ will be
varied. Fig. 3.14 shows the numerical results and the energy curve, and it is found that similar behaviors for Example 3.5 are observed.

In Fig. 3.15, we investigate the effects of fractional diffusion when spinodal decomposition is considered. For $\alpha = 2$ the early stages of phase transition produce a rapid movement to bulk regions of both phases and then motion slows down resulting in the state given at times $t = 25, 50, 100$, respectively. Reducing the fractional power leads to thinner interfaces that allow for smaller bulk regions and a much more heterogeneous phase structure. Furthermore, motion to large bulk regions is dramatically slowed down for fractional models with $\alpha = 1.1, 1.4, 1.7$. This phenomenon is consistent with the finding of [67].

3.5 Concluding remarks

We are concentrated on the numerical maximum principle for several kinds of Allen-Cahn-type equations this chapter, that is, simple Allen-Cahn equations with constant mobility and polynomial free energy, generalized Allen-Cahn equations with nonlinear
Figure 3.14: Example 3.7 with the second-order scheme (3.4.4): (a) numerical solutions; and (b) energy curve. \( \alpha = 1.5 \) and \( \epsilon = 0.02 \), with different time steps \( \tau = 0.5, 1, 1.5 \).

degenerate mobility and logarithmic free energy as well as a given velocity field and fractional-in-space Allen-Cahn equations.

The conventional first-order semi-implicit scheme is adopted for discretization in time for all three equations. For fractional-in-space Allen-Cahn equations, we also study the standard Crank-Nicolson scheme and we prove that this nonlinear second-order scheme can also preserve the maximum principle under reasonable time step constraint. In the spatial space, we use second-order finite difference methods to discretize both the standard Laplace operator and the fractional one. We handle the advection term by the upwinding scheme. Furthermore, we given the point-wise error estimate for the first two equations based on the established numerical maximum principle. In the usual case, it is nontrivial to give a point-wise error estimate due to the lack of numerical maximum principle.
Figure 3.15: Example 3.7. Numerical solutions at a) $t = 25$, b) $t = 50$ and c) $t = 100$ with different fractional derivatives $\alpha = 1.1, 1.4, 1.7, 2$. 
Chapter 4

$L^2$-stability of spectral methods for the Allen-Cahn equation

4.1 Introduction

Energy stability for Allen-Cahn equations has been studied extensively, which has been introduced in the previous chapter. And, in Chapter 3, we have investigated the numerical maximum principle for several Allen-Cahn-type equations. All analysis are based on first-order or second-order finite difference methods in spatial space. However, people will be more interested in high-order schemes preserving the maximum principle, e.g., spectral methods. However, up to authors’ knowledge, there does not exist such works to guarantee the maximum principle for the Allen-Cahn equation.

On the other hand, most attentions are paid to the temporal numerical schemes for Allen-Cahn equations. Recently, some high-order spatial discretization schemes are into consideration for Cahn-Hilliard equations [94, 95], which should be valid for Allen-Cahn equations. In this chapter, we are concerned about the high-order spatial discretizations, i.e. spectral methods. We note that Chen and Shen applied semi-implicit Fourier-spectral method to phase field equations [86], but no rigorous stability analysis was provided. In [87], Liu and Shen offered an $L^2$ stability for a Navier-Stokes system (linear momentum equation) coupled with a Cahn-Hilliard equation (phase field equation). However, the maximum principle can not be preserved by spectral methods even for the simplest linear advection-diffusion equation
Hence, maximum principle is a too strong stability criterion to be satisfied by spectral methods. Some relaxed stability requirement is desired. Next we will prove that Fourier spectral methods can satisfy the $L^2$-stability for the Allen-Cahn equation.

We consider the simple version of the Allen-Cahn equation

$$u_t = \epsilon^2 \Delta u + u - u^3$$  \hspace{1cm} (4.1.1)

with periodic boundary conditions. Here, we define the $L^p$-average norm $||u||_p$ of $u$ in the fixed domain $\Omega$

$$||u||_p = \frac{1}{S_\Omega} ||u||^p_{L^p(\Omega)} = \frac{1}{S_\Omega} \int_\Omega |u|^p \, dx \hspace{1cm} (4.1.2)$$

for even $p$, where $S_\Omega$ is the volume of the domain $\Omega$. By applying the maximum principle, we can obtain a weaker sense maximum principle: $L^p$-stability

$$||u||_p = \frac{1}{S_\Omega} \int_\Omega |u|^p \, dx \leq \frac{1}{S_\Omega} \int_\Omega 1 \, dx = 1, \hspace{1cm} (4.1.3)$$

under the condition that the initial value and the boundary conditions are bounded by the constant 1.

The $L^p$-stability here is essentially $L^p$ uniformly bounded, and, of course, it is weaker than the maximum principle. On the other hand, the uniform $L^p$-stability can derive the maximum principle as $p$ goes to infinity. The larger $p$, the closer $L^p$-stability is to the maximum principle. It is straightforward to design numerical schemes to preserve the uniform $L^p$-stability instead of the overcritical maximum principle. In the following sections, we will show that the Fourier method can only preserve the $L^2$-stability.

### 4.2 $L^p$-stability for continuum equations

In this section, we will establish the $L^p$-stability for continuum Allen-Cahn models for even $p$. To start with, we prove a useful lemma.
Lemma 4.1. For a positive function \( y(t) \), \( y(t) \in C^1([0, +\infty)) \) satisfies
\[
\begin{cases}
\frac{dy}{dt} \leq c(y - y^2), \\
y(0) = y_0,
\end{cases}
\tag{4.2.1}
\]
where \( c \) is a positive constant and \( 0 < y_0 < 1 \). Then
\[
y(t) \leq 1, \quad \forall t \geq 0.
\tag{4.2.2}
\]

Proof. As \( 0 < y(0) < 1 \) and \( y(t) \) is continuous, there exist \( \alpha > 0 \) such that \( y(t) \leq 1, \quad \forall t \in [0, \alpha) \). \( \tag{4.2.3} \)

Assuming the conclusion does not hold, there exist \( t_1 > \alpha \) such that \( y(t_1) > 1 \). Let
\[
\beta = \min \{ t | y(t) = 1 \} \quad \text{and} \quad \exists \delta(t) > 0 \quad \text{s.t.} \quad y(s) > 1 \quad \forall s \in (t, t + \delta(t)). \tag{4.2.4}
\]
It is easy to see \( \alpha \leq \beta < t_1 \), \( y(\beta) = 1 \) and for \( t \in (\beta, \beta + \delta(\beta)] \) we have
\[
y'(t) \leq c(y - y^2) < 0, \tag{4.2.5}
\]
taking the fact that \( y(t) > 1 \) for \( t \in (\beta, \beta + \delta(\beta)) \). Thus
\[
y(\beta + \frac{1}{2} \delta(\beta)) = \int_{\beta}^{\beta + \delta(\beta)/2} y'(s)ds + y(\beta) \\
\leq \int_{\beta}^{\beta + \delta(\beta)/2} c(y(s) - y^2(s))ds + 1 \leq 1.
\tag{4.2.6}
\]
Meanwhile we know \( y(\beta + \frac{1}{2} \delta(\beta)) > 1 \), which leads to a contradiction with (4.2.6). \( \square \)

Before we move on to the main theorem in this section, we will give a clear relation as
\[
\|u\|_p = \frac{1}{S_\Omega} \|u\|_p^p = \frac{1}{S_\Omega} \int_\Omega |u|^pdx = \frac{1}{S_\Omega} \|u^\sharp\|_{L^2}^2. \tag{4.2.7}
\]
Now, we will prove solutions to the continuous model (4.1.1) satisfy the \( L^p \)-stability without using the maximum principle.

Theorem 4.1. Consider the Allen-Cahn problem with periodic or homogeneous Neumann/Dirichlet boundary conditions. If the non-zero initial value \( u_0(x) \in C(\Omega) \) satisfies
\[
\max_{x \in \Omega} |u_0(x)| \leq 1, \tag{4.2.8}
\]

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then the entire solutions satisfy the $L^p$-stability for $p$ is even in the sense that

$$||u(t)||_p \leq 1$$  \hspace{1cm} (4.2.9)

for all $t \geq 0$.

**Proof.** First we will prove that (4.2.9) holds when $p = 2$. Using the boundary conditions and taking $L^2$ inner product of the Allen-Cahn equation (4.1.1) with $u$ yields

$$\frac{1}{2} \frac{d||u||_2^2}{dt} = -\epsilon^2 ||\nabla u||_2^2 + ||u||_2^2 - ||u^3||_2^2,$$  \hspace{1cm} (4.2.10)

where we have taken the fact that $(u, u^3) = ||u^2||_2^2$. Let $p = u^2$ and $q \equiv 1$, then by Cauchy-Schwarz inequality we arrive

$$||u^2||_2^2 = \frac{1}{S_\Omega} |q||_2^2 |p||_2^2 \geq \frac{1}{S_\Omega} (p, q)^2 = \frac{1}{S_\Omega} ||u||_2^2.$$  \hspace{1cm} (4.2.11)

Dividing (4.2.10) by $S_\Omega$ and combining with (4.2.11) gives

$$\frac{d||u(t)||_2^2}{dt} \leq 2(||u(t)||_2^2 - ||u(t)||_2^2).$$  \hspace{1cm} (4.2.12)

Due to non-zero initial value $u_0(x) \in C(\Omega)$ satisfying (4.3.21), we have $0 < ||u(0)||_2 \leq 1$. If $||u(0)||_2 = 1$, $u_0(x) \equiv 1$. Thus we know $u(t, x) \equiv 1$ and $||u(t)||_2 \equiv 1$. For the case $0 < ||u(0)||_2 < 1$, we have

$$||u(t)||_2 \leq 1, \hspace{1cm} \forall t \geq 0$$  \hspace{1cm} (4.2.13)

thanks to the Lemma 4.1. Then we complete the proof by Mathematical Induction for $p > 2$. We assume (4.2.9) holds for $p = 2k - 2$ as $k > 1$, i.e.

$$||u(t)||_{2k-2} = \frac{1}{S_\Omega} ||u^{k-1}||_2^2 \leq 1.$$  \hspace{1cm} (4.2.14)

Next we will prove it still holds for $p = 2k$ based on the case $p = 2k - 2$. Similarly, we take $L^2$ inner product of the Allen-Cahn equation (4.1.1) with $u^{2k-1}$

$$\frac{1}{2k} \frac{d||u||_{2k}^2}{dt} = -\epsilon^2 (2k - 1)||u^{k-1}\nabla u||_2^2 + ||u||_{2k}^2 - (u^3, u^{2k-1}).$$  \hspace{1cm} (4.2.15)
With (4.2.14) the last term in the right-hand side of above equation can be estimated as

\[(u^3, u^{2k-1}) = \|u^{k+1}\|^2 \]
\[\geq \left(\frac{1}{S_\Omega}\|u^{k-1}\|^2\right) \|u^{k+1}\|^2 \]
\[\geq \frac{1}{S_\Omega} (u^{k-1}, u^{k+1})^2 = \frac{1}{S_\Omega} \|u\|_{2k}^2. \tag{4.2.16}\]

Hence, we arrive at

\[\frac{1}{2k} \frac{d\|u\|_{2k}^2}{dt} \leq \|u\|_{2k}^2 - \frac{1}{S_\Omega} \|u\|_{2k}^2. \tag{4.2.17}\]

Dividing (4.2.17) by \(S_\Omega\) gives a similar inequality as (4.2.18)

\[\frac{d\|u(t)\|_{2k}^2}{dt} \leq 2k(\|u(t)\|_{2k}^2 - \|u(t)\|_{2k}^2). \tag{4.2.18}\]

The left can be handled same as for the case when \(p = 2\).

The \(L^p\)-stability is weaker than the maximum principle. However, it is not difficult to see that the \(L^p\)-stability can lead to the maximum principle as \(p\) going to infinity.

### 4.3 Fourier-Galerkin methods and \(L^2\)-stability

**4.3.1 Stability analysis**

In this section, we will investigate the stability of Fourier spectral methods for Allen-Cahn equations with periodic boundary condition. It will be perfect if we can recover the maximum principle by Fourier spectral methods. One natural idea to recover the \(L^p\)-stability for any \(p\). Unfortunately, the Fourier spectral method for Allen-Cahn equations can only preserve the \(L^2\)-stability, which will be showed below.

To demonstrate the main idea, we only consider problems in 1D case, without loss of generality assuming which defined on the domain \([0, 2\pi]\). Actually, our following analysis is suitable for both 2D and 3D cases. For solving the Allen-Cahn equation
by the Fourier spectral method, we seek real solutions \( u_N(t, x) \) in the space \( \hat{B}_N = \text{span}\{e^{inx} | |n| \leq N \} \), i.e.,

\[
  u_N(t, x) = \sum_{|n| \leq N} a_n(t)e^{inx},
\]

(4.3.1)

where the coefficients \( a_n(t) \) are determined by the requirement that the residual

\[
  R_N(t, x) = \partial u_N(t, x) \over \partial t - \left( \epsilon^2 \partial^2 u_N(t, x) \over \partial x^2 + u_N(t, x) - (u_N(t, x))^3 \right),
\]

(4.3.2)
is orthogonal to \( \hat{B}_N \). Same as in the common case, the spectral Fourier projection \( P_N[\omega](x) \) of \( \omega \in L^1[0, 2\pi] \) is given by

\[
  P_N[\omega](x) = \sum_{|n| \leq N} \hat{\omega}(n)e^{inx}, \quad \hat{\omega}(n) := \frac{1}{2\pi} \int_0^{2\pi} \omega(x)e^{-inx} dx.
\]

(4.3.3)

Hence, for the projection operator \( P_N : \hat{B}_M \mapsto \hat{B}_N \) for any \( M \geq N \) we have

\[
  P_N[u_M(x)] = \sum_{|n| \leq N} a_n e^{inx},
\]

(4.3.4)

where \( u_M(x) \in \hat{B}_M \) is given as

\[
  u_M(x) = \sum_{|n| \leq M} a_n e^{inx}.
\]

(4.3.5)

Thus, the requirement \( R_N(t, x) \perp \hat{B}_N \) is equivalent to \( P_N R_N(t, x) = 0 \), i.e.,

\[
  \partial u_N(t, x) \over \partial t = \epsilon^2 \partial^2 u_N(t, x) \over \partial x^2 + u_N(t, x) - P_N[u_N^3(t, x)],
\]

(4.3.6)

for taking the fact that all terms in the residual (4.3.2) belong to \( \hat{B}_N \) except \( u_N^3(t, x) \).

According to (4.1.2), the \( L^2 \)-average norm \( ||u_N(t, x)||_2 \) of \( u_N(t, x) \) is given as

\[
  ||u_N(t, x)||_2 = \frac{1}{2\pi} ||u_N(t, x)||^2 = \frac{1}{2\pi} \int_0^{2\pi} |u_N(t, x)|^2 dx = \sum_{|n| \leq N} |a_n(t)|^2.
\]

(4.3.7)

For the projection operator \( P_N \) we have the following lemma.

**Lemma 4.2.** For the real solution \( u_N(t, x) \) defined by (4.3.37), we have

\[
  (P_N[u_N^3(t, x)], u_N(t, x)) \geq 2\pi ||u_N(t, x)||_2^2.
\]

(4.3.8)
Proof. Denote
\[(u_N(t, x))^3 = \sum_{|n| \leq k} b_n(t) e^{inx},\] (4.3.9)
where \(k = \frac{3N}{2}\), then
\[P_N[u_N^3(t, x)] = \sum_{|n| \leq N/2} b_n(t) e^{inx}.\] (4.3.10)

It is easy to check that
\[(P_N[u_N^3(t, x)], u_N(t, x)) = \sum_{|n| \leq N/2} a_n^*(t) b_n(t),\] (4.3.11)
where \(a_n^*(t)\) means the conjugate of \(a_n(t)\), we using the orthogonality of different basis of \(e^{inx}\), and the inner product \((\cdot, \cdot)\) is the standard inner product as
\[ (f, g) = \int_0^{2\pi} fg^* dx.\] (4.3.12)

As \(u_N(t, x)\) is real, we have the fact that
\[ (u_N^3(t, x), u_N(t, x)) = ||(u_N(t, x))^2||^2_2 = \frac{1}{2\pi} ||1||^2_2 ||u_N^2(t, x)||^2_2 \geq \frac{1}{2\pi} ||u_N^2(t, x), 1||^2_2 = \frac{1}{2\pi} ||u_N(t, x)||^4_2 = 2\pi ||u_N(t, x)||^2_2.\] (4.3.13)

Thus, we get (4.3.8).

\[ \square \]

**Theorem 4.2.** Consider the Allen-Cahn problem with periodic boundary conditions. If the non-zero initial value \(u_0(x) \in C_{\text{per}}(\Omega)\) satisfies
\[ \max_{x \in \Omega} |u_0(x)| \leq 1,\] (4.3.14)
then the entire solutions \(u_N(t, x)\) obtained by the Fourier-Galerkin method satisfy the \(L^2\)-stability in the sense that
\[ ||u_N(t, x)||_2 \leq 1\] (4.3.15)
for all \(t \geq 0\).

Proof. Taking \(L^2\) inner product of equation (4.3.6) with \(u_N(t, x)\) yields
\[ \frac{1}{2} \frac{d}{dt} ||u_N(t, x)||^2_2 = -\varepsilon^2 ||\frac{\partial u_N(t, x)}{\partial x}||^2_2 + ||u_N(t, x)||^2_2 - (P_N[u_N^3(t, x)], u_N(t, x)).\] (4.3.16)
By Lemma 4.2, we have the similar inequality as (4.2.18)

$$\frac{d}{dt}||u_N(t, x)||_2^2 \leq 2(||u_N(t, x)||_2^2 - ||u_N(t, x)||^2).$$  \hspace{1cm} (4.3.17)

We can achieve the conclusion (4.3.15) using the similar analysis process as in Theorem 4.1.

The reason why we can not recover the $L^p$-stability for $p$ greater than 2 is that the Lemma 4.2 does not hold any more in this case. More specifically, the following equality does not hold for $p$ greater than 2

$$(P_N[u_N^3, u_N^{p-1}] = (u_N^3, u_N^{p-1}).$$  \hspace{1cm} (4.3.18)

Though we can not get the $L^p$-stability for $p$ greater than 2, $L^2$-stability can achieve the spectral convergence rate for Allen-Cahn equations.

### 4.3.2 Spectral convergence rate

In this sub-section, we will prove the spectral convergence of Fourier spectral methods for Allen-Cahn equations based on the established $L^2$-stability. We will constraint our consideration in $H^s_{\text{per}}[0, 2\pi]$ space which is equipped with following norm

$$||\omega||^2_{H^q_{\text{per}}} = \sum_{m=0}^{q} \int_0^{2\pi} |\omega^{(m)}(x)|^2 dx.$$  \hspace{1cm} (4.3.19)

For the spectral Fourier projection, we have the point-wise error in the maximum norm as

**Lemma 4.3.** For any $q > 1/2$ and $\omega(x) \in C^q_{\text{per}}[0, 2\pi]$, there exists a positive constant, independent of $N$, such that

$$||\omega - P_N[\omega]||_{\text{max}} \leq CN^{\frac{1}{2} - q}||\omega||_{H^q}.$$  \hspace{1cm} (4.3.20)

For more details, the readers can refer to [60].
Theorem 4.3. Assume the solution of the Allen-Cahn problem (4.1.1) with periodic boundary conditions is sufficiently smooth for \(0 < t \leq T\), specifically, \(u(t, x) \in L^\infty([0, T], H^1_{\text{per}}[0, 2\pi])\). If the non-zero initial value \(u_0(x) \in C^q_{\text{per}}[0, 2\pi]\) satisfies
\[
\max_{x \in \Omega} |u_0(x)| \leq 1,
\] (4.3.21)
then the following convergence rate estimate of the Fourier spectral methods (4.3.6) holds for all \(q > \frac{3}{2}\)
\[
||u_N(t, x) - u(t, x)||_2^2 \lesssim N^{1-2q}||u_0||^2 + N^{\frac{1}{2}-q} \max_{t \leq T} ||u(t, x)||_{H^q} + N^{\frac{3}{2}-q} \max_{t \leq T} ||u^3(t, x)||_{H^q}
\] (4.3.22)
for all \(t \leq T\).

Proof. To simplify notations, denote
\[
E_r(t) = ||u_N(t, x) - u(t, x)||_2^2.
\] (4.3.23)
Then easily calculating yields
\[
\frac{1}{2} \frac{d}{dt} E_r(t) = \int_0^{2\pi} (u_N - u) \frac{\partial}{\partial t} (u_N - u) \, dx
\]
\[
= \int_0^{2\pi} (u_N - u) \left[ \epsilon^2 \frac{\partial^2}{\partial x^2} (u_N - u) + (u_N - u) - (u^3 - P_N[u^3]) \right] \, dx
\] (4.3.24)
\[
\leq ||u_N(t, x) - u(t, x)||_2^2 + \int_0^{2\pi} (u_N - u)(u^3 - P_N[u^3]) \, dx := A(t) + I.
\]
Obviously,
\[
I = \int_0^{2\pi} (u_N - u)(u^3 - P_N[u^3] + P_N[u^3] - P_N[u^3]) \, dx
\]
\[
= \int_0^{2\pi} (u^3 - P_N[u^3])(u_N - u) \, dx + \int_0^{2\pi} (u_N - u)P_N[u^3 - u^3] \, dx := P + Q.
\] (4.3.25)
Since \(u(t, x) \in L^\infty([0, T], H^1_{\text{per}}[0, 2\pi])\), by embedding theorem, we know \(u \in C^q_{\text{per}}[0, 2\pi]\). Hence, \(u^3 \in C^q[0, 2\pi]\). Then, using Lemma 4.3 we get
\[
P \leq ||u^3 - P_N[u^3]||_{L^\infty} \int_0^{2\pi} |u_N - U| \, dx \lesssim N^{\frac{1}{2}-q} ||u||_{H^q} \int_0^{2\pi} |u_N - u| \, dx,
\] (4.3.26)
and
\[
Q = \int_0^{2\pi} (u^3 - u^3) P_N[u_N - u] \, dx = \int_0^{2\pi} (u^3 - u^3)(u_N - u + u - P_N[u]) \, dx
\]
\[
= \int_0^{2\pi} (u - P_N[u])(u^3 - u^3) \, dx - \int_0^{2\pi} (u - u_N)^2(u_N^2 + uu_N + u^2) \, dx
\] (4.3.27)
\[
\leq ||u - P_N[u]||_{L^\infty} \int_0^{2\pi} |u_N^3 - u^3| \, dx \lesssim N^{\frac{1}{2}-q} ||u^3||_{H^q} \int_0^{2\pi} |u_N^3 - u^3| \, dx.
\]
Using Cauchy-Schwartz inequality for \( \int_0^{2\pi} |u_N - u|dx \) we have
\[
\int_0^{2\pi} |u_N - u|dx = (1, |u_N - u|) \leq \sqrt{2\pi} ||u_N - u||_2 \leq \sqrt{2\pi} (||u||_2 + ||u_N||_2) \quad (4.3.28)
\]
Due to the \( L^2 \)-stability for both \( u \) and \( u_N \), \( ||u||_2, ||u_N||_2 \leq \sqrt{2\pi} \). Consequently,
\[
\int_0^{2\pi} |u_N - u|dx \leq 4\pi. \quad (4.3.29)
\]
Note that the \( L^2 \)-stability (4.3.15) is actually equivalent to
\[
||u_N(t, x)||_2 = \sum_{|n| \leq N} |a_n(t)|^2 \leq 1. \quad (4.3.30)
\]
So we know \( |a_n(t)| \leq 1 \). Further more, we have
\[
||u_N(t, x)||_\infty = \max_{x \in [0, 2\pi]} \left| \sum_{|n| \leq N} a_n(t) e^{inx} \right| \leq \sum_{|n| \leq N} |a_n(t)| \lesssim N \quad (4.3.31)
\]
Meanwhile, \( u \) satisfies the maximum principle, that is, \( ||u(t, x)||_\infty \leq 1 \). Then we can estimate
\[
\int_0^{2\pi} |u_N^3 - u^3|dx \leq ||u - u_N||_\infty \int_0^{2\pi} |u_N^2 + uu_N + u^2|dx \lesssim N. \quad (4.3.32)
\]
Hence, \( P \) and \( Q \) can be estimated as
\[
P \lesssim N^{\frac{1}{2} - q} ||u||_{H^q}, \quad Q \lesssim N^{\frac{1}{2} - q} ||u^3||_{H^q}. \quad (4.3.33)
\]
Substituting them into (4.3.24) gives
\[
\frac{d}{dt} E_r(t) \lesssim E_r(t) + N^{\frac{1}{2} - q} ||u||_{H^q} + N^{\frac{1}{2} - q} ||u^3||_{H^q} \quad (4.3.34)
\]
Using Gronwall inequality, we find
\[
E_r(t) \lesssim E_r(0) + N^{\frac{1}{2} - q} \max_{t \leq T} ||u(t, x)||_{H^q} + N^{\frac{3}{2} - q} \max_{t \leq T} ||u^3(t, x)||_{H^q}. \quad (4.3.35)
\]
Moreover, with \( u_N(0, x) = P_N[u_0(x)] \) it follows by Lemma 4.3
\[
E_r(0) = ||u_N(0, x) - u_0(x)||_2^2 \leq 2\pi ||u_0 - P_N[u_0]||_\infty^2 \lesssim N^{1 - 2q} ||u_0||_{H^q}^2. \quad (4.3.36)
\]
Combining (4.3.35) and (4.3.36), we can get the desired result (4.3.22). \( \square \)
4.3.3 A numerical example

In this sub-section we will demonstrate the spectral convergence rate via a numerical example. The solution that we seek has the following form

\[ u_N(t, x) = \sum_{|n| \leq N} a_n(t)e^{inx}. \]  \hspace{1cm} (4.3.37)

Hence, our remaining task is only to compute the Fourier coefficients \( a_n(t) \). The Fourier-Galerkin method (4.3.6) will result in a high nonlinear ordinary differential equation (ODE) system

\[ \frac{d}{dt}A(t) = (I - \epsilon^2 \Lambda)A(t) - H(A(t)), \]  \hspace{1cm} (4.3.38)

where \( I \) is the identity matrix, \( A(t) = (a_{-N}, a_{-N+1}, \cdots, a_{-1}, a_0, a_1, \cdots, a_{N-1}, a_N)^T \), \( \Lambda \) has the following form

\[ \Lambda = \text{diag}(N^2, (N-1)^2, \cdots, 1, 0, 1, \cdots, (N-1)^2, N^2), \]  \hspace{1cm} (4.3.39)

and \( H_j \) of \( H(A(t)) \) is expressed as follows

\[ H_j = \sum_{|p|, |q|, |r| \leq N, p+q+r=j} a_pa_qa_r, \]  \hspace{1cm} (4.3.40)

for \( j = -N, -N+1, \cdots, -1, 0, 1, \cdots, N - 1, N \).

**Example 4.1.** Here, we just take a simple example to verify our analysis for the spectral convergence rate numerically. We consider the one-dimensional Allen-Cahn equation in \([0, 2\pi]\)

\[ u_t = \epsilon^2 \Delta u + u - u^3, \]  \hspace{1cm} (4.3.41)

with periodic boundary conditions and the following initial value

\[ u_0(x) = 0.05 \cos(x). \]  \hspace{1cm} (4.3.42)

We solve the ODE system by the fourth-order Runge-Kutta (RK4) method. We fix \( \epsilon = 0.2 \), time step \( \tau = 0.001 \), terminal time \( T = 1 \). We take solutions by \( N = 64 \) as reference solutions. We plot the point-wise error for \( N = 2, 4, 8 \) in Fig. 4.1. It is observed that the errors decay to zero very rapidly.
Figure 4.1: Point-wise error by RK4 with $\tau = 0.001$ at $T = 1$.

4.4 Fourier-Collocation methods and $L^2$-stability

4.4.1 Semi-discrete equations and $L^2$-stability

The Fourier-Galerkin method (4.3.6) will result in a highly nonlinear ordinary differential system, and it is complicated to apply it for numerical approximations in fully discrete formulation. It is very natural to choose the Fourier collocation method alternatively, which also offers a high accurate discretization tool in spatial space.

We deal with approximations on the Fourier collocation points in $[0, 2\pi]$, i.e., $x_j = \frac{2\pi j}{N}$, $j = 0, 1, \cdots, N - 1$, and we use $u_j^n$ to approximate to $u(t_n, x_j)$, $U^n = (u_0^n, u_1^n, \cdots, u_{N-1}^n)^T$ and $(U^n)^k = ((u_0^n)^k, (u_1^n)^k, \cdots, (u_{N-1}^n)^k)^T$. We semi-discretize the Allen-Cahn equation by the Fourier collocation methods for the space obtaining

$$\left\{ \begin{array}{l}
\frac{dU}{dt} = \epsilon^2 D_h U + U - (U)^3, \\
U(0) = U^0 = (u_0(x_0), u_0(x_1), \cdots, u_0(x_{N-1}))^T,
\end{array} \right. \tag{4.4.1}$$

where $D_h$ is the differential matrix of the second-order derivative associated with Fourier spectral-collocation methods. From [61], for odd $N$ we know $D_h$ satisfies the
following condition

\[ D_h = (D^1)^2, \]  
(4.4.2)

where \( D^1 \) is the differential matrix of the first-order derivative which is circulant and skew-symmetric as \((D^1)^T = -D^1\). And we also define the discrete \( L^2 \)-average norm of \( U \in \mathbb{R}^N \) consistently with (4.1.2) as

\[ \|U\|_2 = \frac{1}{2\pi} \sum_{j=0}^{N-1} \frac{2\pi}{N} |u_j|^2 = \frac{1}{N} \sum_{j=0}^{N-1} |u_j|^2 = \frac{1}{N} \|U\|_2^2. \]  
(4.4.3)

Now we can establish the \( L^2 \)-stability in the semi-discrete form given in the following theorem.

**Theorem 4.4.** Consider the semi-discretized Allen-Cahn problem (4.4.1). If the non-zero initial value \( U^0 \) satisfies

\[ \|U^0\|_\infty \leq 1, \]  
(4.4.4)

then the entire solutions satisfy the \( L^2 \)-stability in the sense that

\[ \|U(t)\|_2 \leq 1 \]  
(4.4.5)

for all \( t \geq 0 \).

**Proof.** Taking \( L^2 \) inner product of (4.4.1) with \( U^T \) yields

\[ \frac{1}{2} \frac{d\|U\|_2^2}{dt} = \epsilon^2 U^T D_h U + \|U\|_2^2 - \|(U)^2\|_2^2, \]  
(4.4.6)

where we also take the fact that \( U^T (U)^3 = \|(U)^2\|_2^2 \). We claim \( \epsilon^2 U^T D_h U \leq 0 \) as

\[ \epsilon^2 U^T D_h U = \epsilon^2 U^T (D^1)^2 U = \epsilon^2 U^T D^1 D^1 U = \epsilon^2 (D^1 U)^T (D^1 U) = -\epsilon^2 \|D^1 U\|_2^2 \leq 0, \]  
(4.4.7)

If we take \( P = (1, 1, \ldots, 1)^T \) and \( Q = (U_0, U_1, \ldots, U_{N-1}) \), we can also get similar inequality as (4.2.11)

\[ \|(U)^2\|_2^2 = \frac{1}{N} \|P\|_2^2 \|Q\|_2^2 \geq \frac{1}{N} \|P^T Q\|^2 = \frac{1}{N} \|P\|_2^2 \|Q\|_2^2. \]  
(4.4.8)

The left is quite similar with the analysis in the Theorem (4.1), so we omit it here. \( \square \)
4.4.2 Operator splitting methods

We adopt the operator splitting method to solve the semi-discretized Allen-Cahn equation

\[ \begin{cases} \frac{dU}{dt} = \epsilon^2 D_h U + U - (U)^3, \\ U(0) = U^0 = (u_0(x_0), u_0(x_1), \cdots, u_0(x_{N-1}))^T. \end{cases} \] (4.4.9)

We first split the above ODEs into two sub-problems as following

\[ A : \quad \frac{dV}{dt} = V - (V)^3, \] (4.4.10)

and

\[ B : \quad \frac{dW}{dt} = \epsilon^2 D_h W. \] (4.4.11)

To keep the presentation short, we denote \( S_A^t V_0 \) to represent the Problem A processing time \( t \) with initial value \( V_0 \). Taking the similar notation in [64], we can obtain high order splitting methods in form

\[ U^{n+1} = P_s U^n = \prod_{j=1}^{s} S_{b_j \tau} S_{a_j \tau} U^n = S_{b_1 \tau} S_{a_1 \tau} S_{b_2 \tau} S_{a_2 \tau} \cdots S_{b_s \tau} S_{a_s \tau} U^n, \] (4.4.12)

where \( \tau \) is the time step. For example, when \( s = 2 \), \( a_1 = a_2 = 0.5 \), \( b_1 = 1 \) and \( b_2 = 0 \), this is the famous second order Strang splitting given in [62] as

\[ U^{n+1} = P_2 U^n = S_{\frac{\tau}{2}} S_{\frac{\tau}{2}} S_{a_1 \tau} S_{a_1 \tau} U^n. \] (4.4.13)

In [64], Blanes and Moan proposed the fourth order scheme involving coefficients \( a_j, b_j \in R, 1 \leq j \leq s = 7 \) which given in the Table 4.1. Higher order even sixth order or eighth order splitting schemes can be found in [64]. Theoretically, we can obtain arbitrary high order scheme by this kind of splitting.

The two sub-problems: Problem A and Problem B can be solved analytically whose solutions are given respectively as following

\[ v^{n+1}_j = S^A v^n_j = \frac{v^n_j}{\sqrt{e^{-2\tau} + (1 - e^{-2\tau})(v^n_j)^2}}, \quad j = 0, 1, \cdots, N-1, \] (4.4.14)
Problem A and

\[ W^{n+1} = S^B_t W^n = e^{\tau^2 D_h} W^n, \]  

(4.4.15)

to Problem B. The computation in (4.4.14) is point-wise computing which just cost \( O(N) \) operations. However, it will need much more effort to calculate the matrix exponential in the general case. That is the reason why people prefer to handle this kind of linear ODE system by such as Runge-Kutta (RK) schemes other than exponential matrix methods. Fortunately, the differential matrix \( D_h \) is a circulant matrix. Next, we will apply FFT to handle the computation in (4.4.15) which will just cost \( O(N \log_2 N) \) operations. What is more benefit is that the Problem B is solved exactly in time.

So our next goal is to compute \( e^{D} W \) super fast by FFT and \( D \) is an arbitrary circulant matrix. All properties involved to the circulant matrix here can be found in [82]. The unitary discrete Fourier transform (DFT) matrix \( V_N \) is given as

\[ V_N = \frac{1}{\sqrt{N}} F_N, \]

where \( F_N = (f_{jk}) \) with \( f_{jk} = e^{-2jki/N} \), for \( 0 \leq j, k < N \), in fact, \( F_N \) is the exact DFT matrix. Thus, we can decompose \( D \) by \( V_N \) as

\[ D = V_N^* \text{diag}(F_N d) V_N = \frac{1}{N} F_N^* \text{diag}(F_N d) F_N, \]  

(4.4.16)

where \( d \) is the first column of \( D \) and \( \text{diag}(c) \) means forming a diagonal matrix by the vector \( c \). Since \( V_N \) is a unitary matrix, we can easily get the form of \( e^{D} W \) as

\[ e^{D} = V_N^* e^{\text{diag}(F_N d)} V_N W = \frac{1}{N} F_N^* e^{\text{diag}(F_N d)} F_N W. \]  

(4.4.17)
Taking the fact that $\frac{1}{N}F_N^* \text{ is the inverse DFT matrix,}$ the above computing can be implemented in Matlab code succinctly
\[
eDW=\text{real}(\text{ifft}(\exp(\text{fft}(d)) \cdot \text{fft}(W))),
\]
where $\text{fft}$ and $\text{ifft}$ represent FFT and inverse FFT respectively. Obviously, the total operations are the same order of the computation involved in FFT and inverse FFT which is $O(N\log_2 N)$.

### 4.4.3 Fully discretized schemes using second-order splitting

In this section, we will prove that the second order splitting methods defined as (4.4.13) can inherit the $L^2$-stability defined by (4.1.3) in the full discretization. Here, the discrete form of $L^2$-average is defined consistently with (4.1.3) as
\[
\overline{U} = \frac{1}{2\pi} ||U||^2 = \frac{1}{2\pi} \sum_{j=0}^{N-1} \frac{2\pi}{N} |u_j|^2 = \frac{1}{N} \sum_{j=0}^{N-1} |u_j|^2.
\] (4.4.18)

In the following lemmas, our only assumption imposed on the initial value $U^0 = (u_0(x_0), u_0(x_1), \cdots, u_0(x_{N-1}))^T$ is that
\[
\overline{u_0} = \frac{1}{N} \sum_{j=0}^{N-1} |u_0(x_j)|^2 \leq 1.
\] (4.4.19)

For simplicity, we denote $\theta = e^{-2\tau}$, where $0 < \theta < 1$ as $\tau > 0$.

**Lemma 4.4.** The Problem A with initial value $V^0$ is presented as
\[
\begin{cases}
\frac{dV}{d\tau} = V - (V)^3, \\
V(0) = V^0 = (v_0^0, v_1^0, \cdots, v_{N-1}^0)^T
\end{cases}
\] (4.4.20)

Assume the initial value $V^0$ satisfies the assumption (4.4.19), then the entire solution $V(\tau)$ satisfies the $L^2$-stability
\[
\overline{V(\tau)} = \overline{S_\tau^A V^0} \leq 1
\] (4.4.21)

for any time $\tau > 0$. 


Proof. By (4.4.14), we have

\[
||V(\tau)||_2^2 = ||S^A_{\tau}V^0||_2^2 = \sum_{j=0}^{N-1} \frac{|v_j^0|^2}{\theta + (1-\theta)|v_j^0|^2}.
\]  

(4.4.22)

We introduce a function \( g(\alpha) \) defined as

\[
g(\alpha) = \frac{\alpha}{\theta + (1-\theta)\alpha}, \quad \text{for} \quad \alpha \in [0, \infty).
\]  

(4.4.23)

Simply calculating yields

\[
g'(\alpha) = \frac{\theta}{[\theta + (1-\theta)\alpha]^2}, \quad g''(\alpha) = \frac{-2\theta(1-\theta)}{[\theta + (1-\theta)\alpha]^3}.
\]  

(4.4.24)

It is easy to observe that \( g'(\alpha) > 0 \) and \( g''(\alpha) < 0 \) for \( \alpha \geq 0 \) as \( 0 < \theta < 1 \). So \( g(\alpha) \) is a monotone-increasing concave function in \([0, +\infty)\). Denote \( \alpha_j = |v_j^0|^2 \) for \( j = 0, 1, \cdots, N - 1 \). Thus

\[
\overline{V}^0 = \frac{1}{N} \sum_{j=0}^{N-1} \alpha_j \leq 1 \quad \text{and} \quad \overline{V}(\tau) = \frac{1}{N} \sum_{j=0}^{N-1} g(\alpha_j).
\]  

(4.4.25)

Since \( g(\alpha) \) is a monotone-increasing concave function in \([0, +\infty)\), we get

\[
\overline{V}(\tau) = \frac{1}{N} \sum_{j=0}^{N-1} g(\alpha_j) \leq g\left(\frac{1}{N} \sum_{j=0}^{N-1} \alpha_j\right) \leq g(1) = 1,
\]  

(4.4.26)

which holds for any \( \tau > 0 \).

Lemma 4.5. The Problem B with initial value \( W^0 \) is presented as

\[
\begin{cases}
\frac{dW}{dt} = \epsilon^2 D_h W; \\
W(0) = W^0 = (w_0^0, w_1^0, \cdots, w_{N-1}^0)^T
\end{cases}
\]  

(4.4.27)

The entire solution \( W(\tau) \) is bounded by the initial value as

\[
||W(\tau)||_2^2 = ||S^B_{\tau}W^0||_2^2 \leq ||W^0||_2^2
\]  

(4.4.28)

for any time \( \tau > 0 \).

Proof. The whole proof can be found in [60] \( \square \)
Consequently, if the initial value $W^0$ satisfies the assumption (4.4.19), we can get
\[ W(\tau) = S^2_{\tau}W^0 \leq W^0 \leq 1. \] (4.4.29)

Based on the preliminary Lemma 4.4-4.5, we achieve the key theorem of this paper straightforwardly.

**Theorem 4.5.** Consider the Allen-Cahn problem with periodic boundary conditions. If the initial value is bounded by \(1\), i.e., \(\max_{x \in \Omega} |u_0(x)| \leq 1\), then solutions obtained by the fully discrete Strang splitting method defined as (4.4.13) satisfies the $L^2$-stability in the sense that
\[ U^n = (P_2)^nU^0 = (S^A_\tau S^B_\tau S^A_\tau)^nU^0 \leq 1 \] (4.4.30)
for all \(n > 0\) with positive time step $\tau$.

We should pay extra attention to the positive time step constraint on each subproblem. Unfortunately, in [65], Suzuki has proved that, beyond second order, any splitting scheme in (4.4.12) must contain negative coefficients in the set \(\{a_j, b_j\}\). Consequently, our stability analysis only holds for second order splitting scheme. However, in the practice simulations, we find the numerical results by the fourth order splitting scheme are quite satisfied though the stability analysis does not hold, which will be showed in the next section. The $L^2$-stability (4.4.30) is equivalent to
\[ ||U^n||_2^2 = \sum_{j=0}^{N-1} |u^n_j|^2 \leq N, \] (4.4.31)
from which we can get a bound in $L^\infty$ norm as
\[ ||U^n||_\infty = \max_j |u^n_j| \leq \sqrt{N}, \] (4.4.32)
which is independent on time level $n$.

### 4.4.4 Numerical tests

In this section, we present some numerical experiments to verify the theoretical results obtained in the previous sections. Since our analysis is independent of dimensions,
for simplicity we only consider one-dimensional problems with periodic boundary condition.

**Example 4.2.** The initial condition is chosen as

\[ u_0(x) = 0.05 \sin(x). \]

The parameter \( \epsilon^2 \) is 0.01, the computation domain is \([0, 2\pi]\) and the mesh size in space is \( h = \frac{\pi}{64} \). We take solutions obtained by RK4 methods with very small time step \( \tau = 0.001 \) as reference solutions to test convergence rate.

For the second order splitting method, we take the Strang splitting and, for the fourth order splitting method, we take the scheme as given in Table 4.1. The results are showed in Table 4.2 and Table 4.3.

<table>
<thead>
<tr>
<th>Order</th>
<th>( \tau = 0.2 )</th>
<th>( \tau = 0.1 )</th>
<th>( \tau = 0.05 )</th>
<th>( \tau = 0.025 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2nd</td>
<td>Error 5.88e-7</td>
<td>1.47e-7</td>
<td>3.69e-8</td>
<td>9.23e-9</td>
</tr>
<tr>
<td></td>
<td>Rate -</td>
<td>1.995</td>
<td>1.999</td>
<td>2.000</td>
</tr>
<tr>
<td>4th</td>
<td>Error 6.68e-11</td>
<td>4.19e-12</td>
<td>2.54e-13</td>
<td>1.69e-14</td>
</tr>
<tr>
<td></td>
<td>Rate -</td>
<td>3.997</td>
<td>4.040</td>
<td>3.910</td>
</tr>
<tr>
<td>RK4</td>
<td>Error 9.92e-7</td>
<td>6.72e-8</td>
<td>4.37e-9</td>
<td>2.79e-10</td>
</tr>
<tr>
<td></td>
<td>Rate -</td>
<td>3.884</td>
<td>3.942</td>
<td>3.971</td>
</tr>
</tbody>
</table>

Table 4.2: Errors and convergence rate at \( T = 1 \) compared with reference solutions.

<table>
<thead>
<tr>
<th>Order</th>
<th>( \tau = 0.2 )</th>
<th>( \tau = 0.1 )</th>
<th>( \tau = 0.05 )</th>
<th>( \tau = 0.025 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2nd</td>
<td>Error 6.27e-3</td>
<td>1.59e-3</td>
<td>3.98e-4</td>
<td>9.95e-5</td>
</tr>
<tr>
<td></td>
<td>Rate -</td>
<td>1.984</td>
<td>1.996</td>
<td>1.999</td>
</tr>
<tr>
<td>4th</td>
<td>Error 5.48e-7</td>
<td>2.77e-8</td>
<td>1.61e-9</td>
<td>9.90e-11</td>
</tr>
<tr>
<td></td>
<td>Rate -</td>
<td>4.308</td>
<td>4.104</td>
<td>4.024</td>
</tr>
</tbody>
</table>

Table 4.3: Errors and convergence rate at \( T = 10 \) compared with reference solutions.
From two tables, we can see the numerical scheme can achieve the optimal convergence rate. Compared two splitting schemes with each other, the fourth order splitting scheme are much more accurate than the second order scheme. Furthermore, we can observe that, as fourth order schemes, the fourth order splitting scheme can enhance the accuracy much more than RK4, which indicates that the truncation error of the former one is much smaller than the one of the latter.

Figure 4.2: Solutions with fourth order Runge-Kutta methods.

We now study the performance of two splitting schemes with large time step to achieve the steady state. We will use the $L^2$-average defined by (4.4.18) to measure the robustness of schemes. We also use the same example as above. First, we get a reference solution at $T = 100$ by RK4 with small time step $\tau = 0.01$. But if we take time step nine times bigger as $\tau = 0.1$ by RK4, the $L^2$ norm blows up at just $T = 3$, which is presented in Fig. 4.2. On the other hand, we can find the splitting schemes make larger time step allowed.

In Fig. 4.3, we observe that both two schemes work quite well to achieve the steady state with $\tau = 0.5$ and the $L^2$-average is uniformly bounded by 1. But when we enlarge the time step to $\tau = 2$ (showed in Fig. 4.4), the second order splitting scheme seems the same with naked eyes. However, the fourth order splitting scheme gets the totally wrong solutions. In unpresented experiments, we observe that the second order splitting scheme can guarantee the $L^2$-stability even when $\tau = 100$ which is in good agreement with the results of Theorem 4.5, but the fourth order schemes blow up very fast.
Figure 4.3: Solutions at $T = 100$ with $\tau = 0.5$ by two splitting schemes.

Figure 4.4: Solutions at $T = 100$ with $\tau = 2$ by two splitting schemes.

In all, the fourth order scheme can resolve the solutions much better with relative small time step, such as the results are quite satisfied when $\tau = 0.2$ (see in above tables). But if we are more interested in the steady state, the second order splitting
scheme are more reliable.

### 4.5 Concluding remarks

In this chapter, we proposed a new stability for the Allen-Cahn equation: $L^p$-stability which is a new stability criterion unlike the nonlinear energy stability and the maximum principle. We have showed that the $L^2$-stability can be preserved by both Fourier spectral Galerkin methods and Fourier spectral collocation methods. Meanwhile, we adopt the operator splitting method in time and Fourier-collocation method for spatial space to simulate the Allen-Cahn equation in fully discrete form. We prove that the Strang splitting scheme can guarantee the $L^2$-stability.

We also believe that the similar results can be obtained by Chebyshev spectral methods or Legendre spectral methods. In the following work, we are interested in designing high order time discretization schemes to preserve the $L^2$-stability, and numerical schemes satisfy the $L^p$-stability for larger $p$ is also a meaningful work. Since the larger $p$ the closer we achieve the maximum principle.
Chapter 5

Long time simulations with $p$-adaptivity

5.1 Introduction

In this chapter, we will address to long time simulations of three phase-field models, namely, the Allen-Cahn equation (ACE):

\[
\frac{\partial u}{\partial t} = \epsilon^2 \Delta u - f(u), \quad x \in \Omega, \ t \in (0, T],
\]

\[
u(x, 0) = u_0(x), \quad x \in \bar{\Omega};
\] (5.1.1)

the Cahn-Hilliard equation (CHE):

\[
\frac{\partial u}{\partial t} = \Delta(-\epsilon^2 \Delta u + f(u)), \quad x \in \Omega, \ t \in (0, T],
\]

\[
u(x, 0) = u_0(x), \quad x \in \bar{\Omega};
\] (5.1.3)

and the thin film model (TFM) (also called molecular beam epitaxy model):

\[
\frac{\partial u}{\partial t} = -\epsilon^2 \Delta^2 u + \nabla \cdot f(\nabla u), \quad x \in \Omega, \ t \in (0, T],
\]

\[
u(x, 0) = u_0(x), \quad x \in \bar{\Omega}.
\] (5.1.5)

For simplicity, we impose periodic boundary conditions or homogeneous Neumann boundary conditions for all of the three equations. Here $\Omega$ is a bounded domain in $\mathbb{R}^2$ and $T$ is a finite time.

Since we have given some details about the first two equations, we next only give brief introduction on the thin film model. In the thin film model (5.1.5), $u$ is a scaled
height function of epitaxial growth of thin films in a co-moving frame. It can be viewed as a $L^2$ gradient flow associated with the following energy functional

$$E(u) = \int_\Omega \left( \frac{1}{2} \epsilon^2 |\Delta u|^2 + F(\nabla u) \right) dx$$  \hspace{1cm} (5.1.7)$$

There are two common choices in the nonlinear term, that is, with slope selection

$$F(\nabla u) = \frac{1}{4} (|\nabla u|^2 - 1)^2, \quad f(\nabla u) = -(1 - |\nabla u|^2) \nabla u,$$  \hspace{1cm} (5.1.8)$$

and without slope selection

$$F(\nabla u) = -\frac{1}{2} \ln(|\nabla u|^2 + 1), \quad f(\nabla u) = -\frac{\nabla u}{1 + |\nabla u|^2}.$$ \hspace{1cm} (5.1.9)$$

Due to no available analytical solutions for thin film models, numerical simulations and numerical analysis have been studied extensively. For temporal discretization, the numerical methods can be classified into explicit schemes (linear schemes), implicit schemes (nonlinear schemes), and implicit-explicit schemes. In general, the implicit-explicit approach is found more powerful in terms of accuracy and stability. Xu and Tang proposed an stabilized semi-implicit scheme to guarantee the energy stability for the thin film model with slope selection [42], in which a nonlinear relationship between the added stabilized parameter and the numerical solutions are derived. Furthermore, in [58], Tang et al. adopted a second-order nonlinear scheme to simulate this model via an adaptive time-stepping strategy. Based on the energy convex splitting technique [39], Wang et al. accomplished several works on thin film models both with slope selection and without slope selection [41, 76, 77, 78], in which both first-order linear and nonlinear schemes as well as second-order nonlinear schemes are considered.

As the governing equations (5.1.3) and (5.1.5) involve the perturbed (i.e., the coefficient $\epsilon^2 \ll 1$) biharmonic operators and strong nonlinearities, it is very difficult to design efficient time discretization strategy which can resolve dynamics and steady state of the corresponding phase field models. Moreover, nonlinear energy
stability which is intrinsic to the phase field models (see, e.g., Fig. 5.1) is also a challenging issue for numerical approximations. Numerical evidences show that violating the energy stability may lead to non-physical oscillations. Consequently, a satisfactory numerical strategy needs to balance solution accuracy, efficiency and nonlinear stability.

![Illustrative energy curves of the three different models.](image)

Among the time discretizations concerning nonlinear stability, Eyre’s [39] convex splitting scheme should be specially mentioned. It is a first-order accurate unconditionally stable time-stepping scheme for gradient flows, which can be either linear or nonlinear depending on the ways of splitting. In particular, it has served as inspiration for many other time integration schemes in recent years. The starting point of our work is also based on the convex splitting scheme. Moreover, explicit schemes may have stability problems and fully nonlinear schemes require nonlinear iterations at each time step. As we are interested in both small and large time scale dynamics, the linear implicit-explicit schemes are into our consideration. More precisely, we will first consider a linear implicit-explicit scheme by using the convex splitting idea.

Below we will briefly outline the motivation and main findings of this work. Our numerical evidences show that the lower order time discretizations may require very small time stepsizes in order to resolve the short time dynamics of the phase field problems. Fig. 5.2 gives a typical example which shows energy evolutions for the Cahn-Hilliard problem (5.1.3)-(5.1.4) with $\Delta t = 1/1000, 1/100, 1/50$. It is observed that a time step smaller than $10^{-2}$ is needed in order to obtain accurate solutions.
For improvement, one quick idea is to use higher order time discretization. However, there has no higher order energy-stable schemes, particularly for order 3 or higher. Our idea is to use the so-called spectral deferred correction (SDC) method which was first introduced to solve initial value ordinary differential equations (ODEs) by Dutt, Greengard and Rokhlin [79]. The key idea of the SDC method is to first convert the original ODEs into the corresponding Picard equation and then apply a deferred correction procedure in the integral formulation, aiming to achieve higher order accuracy in an iterative way. We also note that SDC methods are applied to simulate Allen-Cahn equations and Cahn-Hilliard equations in [63]. The reasons for us to employ the SDC method are the following: iteration loops can improve the formal accuracy in an flexible and simple way; the SDC method was designed to handle stiff systems which are the case of our perturbed singularly nonlinear equations; and the flexibility of the order enhancement is useful for our local adaptive strategy to be described later. On the other hand, although the SDC method can solve the short-time dynamics very well (e.g., a 5th-order time discretization can fix the problem in

Figure 5.2: A typical example for the energy dependent on time steps for the Cahn-Hilliard equation. The detail description of the example can be found in Section 6.
Fig. 5.2 with $\Delta t = 1/20$), unfortunately, a higher order time discretization may yield numerical instability as the nonlinear stability can not be guaranteed for higher order time discretizations. A typical example is given in Fig. 5.3, which solves the same example as in Fig. 5.2 but with a 3rd order SDC method (i.e. $Np = 2$ in the figure) and an 5th-order SDC method (i.e. $Np = 4$). It is observed that the discrete energies blow up before $T = 30$. To fix the problems in Figs. 5.2 and 5.3 above, we will propose a hybrid $p$-adaptive method which chooses appropriate order of accuracy at each time level. It is seen from the energy curves in Fig. 5.1 that first-order methods should be good enough in most of time regimes, but in some critical stages with rapid energy change appropriate adaptive strategies must be used. Some $p$-adaptive details will be reported and the relevant numerical results will be presented in this work. It will be demonstrated that the adaptive procedure is robust and effective for simulating both dynamics and steady state of the phase field problems.

**5.2 Energy stability**

Below we will give three energy stable schemes for Allen-Cahn equations, Cahn-Hilliard equations and thin film models respectively. These three schemes can be
viewed as linearization of energy convex splitting technique, but, as an individual, all of them are studied in [43], [42] and [77] respectively. Here we follow their main idea with some supplementation or generalization.

### 5.2.1 Allen-Cahn equations

We will use the following temporal scheme for Allen-Cahn equations with time step $k$ is given by

$$\frac{u^{n+1} - u^n}{k} = \varepsilon^2 \Delta u^{n+1} - \beta u^{n+1} + \beta u^n - f(u^n). \quad (5.2.1)$$

**Theorem 5.1.** For the Allen-Cahn equation with boundary values and initial values which are both bounded by 1, the semi-discrete scheme (5.2.1) with

$$\beta + \frac{1}{k} \geq 2 \quad (5.2.2)$$

is unconditionally energy stable, i.e.,

$$E(u^{n+1}) \leq E(u^n), \quad n = 0, 1, \cdots \quad (5.2.3)$$

**Proof.** The stabilized scheme (5.2.1) can be concisely rewritten as

$$(1 + \beta k)u^{n+1} - k\varepsilon^2 \Delta u^{n+1} = (1 + \beta k)u^n + k(u^n - (u^n)^3), \quad (5.2.4)$$

where we have used the fact that $f(u) = u - u^3$. Denote

$$g(x) = (1 + \beta k)x + k(x - x^3). \quad (5.2.5)$$

Under condition (5.2.2), it is easy to check the following conclusion

$$\max_{|x| \leq 1} g(x) = g(1) = 1 + \beta k; \quad \min_{|x| \leq 1} g(x) = g(-1) = -(1 + \beta k), \quad (5.2.6)$$

By Mathematical Induction if we assume $\|u^n\|_\infty \leq 1$, we find

$$\|g(u^n)\|_\infty \leq 1 + \beta k. \quad (5.2.7)$$

If $u^{n+1}(x)$ achieves the maximum at $x^*$ inside $\Omega$, then at this point,

$$\Delta u^{n+1}(x^*) \leq 0. \quad (5.2.8)$$
Hence
\[(1 + \beta k) \max(u^{n+1}) \leq g(u^n(x^*)). \tag{5.2.9}\]
Similarly, we can get
\[(1 + \beta k) \min(u^{n+1}) \geq g(u^n(x^{**})). \tag{5.2.10}\]
Since the boundary values are bounded by 1, we find
\[(1 + \beta k) \| u^{n+1} \|_\infty \leq \| g(u^n) \|_\infty \leq 1 + \beta k. \tag{5.2.11}\]
So far, we know that both \(u^n(x)\) and \(u^{n+1}(x)\) are bounded by 1 if the initial values are bounded by 1. Taking the energy difference between two consecutive time levels and expanding \(F(u)\) by Taylor expansion yield
\[
E(u^{n+1}) - E(u^n) = \frac{\epsilon^2}{2} \left( \| \nabla u^{n+1} \|^2 - \| \nabla u^n \|^2 \right) + (f(u^n), u^{n+1} - u^n) + \frac{1}{2} (f'(\xi_n)(u^{n+1} - u^n), u^{n+1} - u^n),
\]
where \(f'(\xi_n) = 1 - 3\xi_n^2\) and \(\xi_n\) lies between \(u^n\) and \(u^{n+1}\). Furthermore, we have \(\xi_n \in [-1, 1]\). Hence, we get \(|f'(\xi_n)| \leq 2\). Consequently, (5.2.12) can be estimated as
\[
E(u^{n+1}) - E(u^n) \leq \frac{\epsilon^2}{2} \left( \| \nabla u^{n+1} \|^2 - \| \nabla u^n \|^2 \right) + (f(u^n), u^{n+1} - u^n) + \| u^{n+1} - u^n \|^2. \tag{5.2.13}\]
Taking \(L^2\) inner product of (5.2.1) with \(u^{n+1} - u^n\), we get
\[
\frac{\| u^{n+1} - u^n \|^2}{k} = \epsilon^2 (\Delta u^{n+1}, u^{n+1} - u^n) - \beta \| u^{n+1} - u^n \|^2 - (f(u^n), (u^{n+1} - u^n)) =: I_1 - \beta \| u^{n+1} - u^n \|^2 - (f(u^n), u^{n+1} - u^n). \tag{5.2.14}\]
It can be shown that
\[
I_1 = -\frac{\epsilon^2}{2} \left( \| \nabla u^{n+1} \|^2 - \| \nabla u^n \|^2 + \| \nabla u^{n+1} - \nabla u^n \|^2 \right). \tag{5.2.15}\]
Substituting \(I_1\) back into (5.2.14), then
\[
-\frac{\epsilon^2}{2} \| \nabla u^{n+1} - \nabla u^n \|^2 \tag{5.2.16}
\]
\[
= \frac{\epsilon^2}{2} (\| \nabla u^{n+1} \|^2 - \| \nabla u^n \|^2) + \| \nabla u^{n+1} - u^n \|^2 + (f(u^n), u^{n+1} - u^n).\]
Combining (5.2.13) and (5.2.16) and using the condition (5.2.2), we have

$$E(U^{n+1}) - E(U^n) \leq -\frac{\epsilon^2}{2} ||\nabla u^{n+1} - \nabla u^n||^2_2 - (\beta + \frac{1}{k} - 1)||u^{n+1} - u^n||^2_2. \quad (5.2.17)$$

Then we complete the proof by the condition (5.2.2).

The above result seems new in the sense that the constant $\beta$ can be bounded uniformly by using the maximum principle for the semi-discrete scheme. This makes the splitting scheme (5.2.1) theoretically reliable.

### 5.2.2 Cahn-Hilliard equations

For the Cahn-Hilliard equation, we use the stabilized semi-implicit scheme

$$\frac{u^{n+1} - u^n}{k} = -\epsilon^2 \Delta^2 u^{n+1} + \beta \Delta u^{n+1} - \beta \Delta u^{n} + \Delta f(u^n). \quad (5.2.18)$$

**Theorem 5.2.** For the Cahn-Hilliard equation, if the constant $\beta$ in (5.2.18) is sufficiently large then the semi-discrete scheme (5.2.18) is unconditionally energy stable, i.e.,

$$E(u^{n+1}) \leq E(u^{n}), \quad n = 0, 1, \cdots \quad (5.2.19)$$

Moreover, if the numerical solution is convergent in $L^\infty([0,T], W^{1,\infty}(\Omega))$ as $k \to 0$, then the size of the constant $\beta$ can be controlled by

$$\beta \geq \frac{1}{2} \max \{ \|f'(v)\|_\infty, \|f'(\xi_n)\|_\infty, 1 \}. \quad (5.2.20)$$

**Proof.** Taking the energy difference between two consecutive time levels and expanding $F(u)$ by Taylor expansion yield

$$E(u^{n+1}) - E(u^n) = \frac{\epsilon^2}{2} \left( ||\nabla u^{n+1}||^2_2 - ||\nabla u^n||^2_2 \right) + (f(u^n), u^{n+1} - u^n) + \frac{1}{2} \left( f'({\xi_n})(u^{n+1} - u^n), u^{n+1} - u^n \right) \leq \frac{\epsilon^2}{2} \left( ||\nabla u^{n+1}||^2_2 - ||\nabla u^n||^2_2 \right) + (f(u^n), u^{n+1} - u^n) + \frac{\alpha_n}{2} ||u^{n+1} - u^n||^2_2, \quad (5.2.21)$$

where

$$\alpha_n := \max \left\{ \|f'(u^n)\|_\infty, \|f'(u^{n+1})\|_\infty, 1 \right\}. \quad (5.2.22)$$
Rewrite the scheme (5.2.18) as
\[ u^{n+1} - u^n = k \Delta \eta, \]  
(5.2.23a)
\[ \eta = -\epsilon^2 \Delta u^{n+1} + \beta u^{n+1} - \beta u^n + f(u^n). \]  
(5.2.23b)

Assume that
\[ \beta \geq \frac{1}{2} \alpha_n. \]  
(5.2.24)

Taking \( L^2 \) inner product for (5.2.23a) with \( \eta \) and combining (5.2.21) yields
\[ (\eta, u^{n+1} - u^n) = -k ||\nabla \eta\||^2_2 \]
\[ = (-\epsilon^2 \Delta u^{n+1} + \beta u^{n+1} - \beta u^n + f(u^n), u^{n+1} - u^n) \]
\[ = \epsilon^2 (\nabla u^{n+1}, \nabla u^{n+1} - \nabla u^n) + \beta ||u^{n+1} - u^n||^2_2 + (f(u^n), u^{n+1} - u^n) \]
\[ \geq \frac{\epsilon^2}{2} (||\nabla u^{n+1}||^2_2 - ||\nabla u^n||^2_2) + \frac{\alpha_n}{2} ||u^{n+1} - u^n||^2_2 + (f(u^n), u^{n+1} - u^n) + \frac{\epsilon^2}{2} ||u^{n+1} - u^n||^2_2 \]
\[ \geq E(u^{n+1}) - E(u^n) + \frac{\epsilon^2}{2} ||\nabla u^{n+1} - \nabla u^n||^2_2, \]
where in the second last step we have used (5.2.24). Consequently, we have
\[ E(u^{n+1}) - E(u^n) \leq -k ||\nabla \eta\||^2_2 - \frac{\epsilon^2}{2} ||\nabla u^{n+1} - \nabla u^n||^2_2 \leq 0, \]
which is the desired result (5.2.19). If the numerical solution is convergent in \( L^\infty([0, T], W^{1,\infty}(\Omega)) \) as \( k \to 0 \), then combining (5.2.22) and (5.2.24) gives (5.2.20).

\[ \Box \]

5.2.3 Thin film models

We consider thin film models both with slope selection and without slope selection as a united in a general form
\[ \frac{u^{n+1} - u^n}{k} = -\epsilon^2 \Delta^2 u^{n+1} + \beta \Delta u^{n+1} - \beta \Delta u^n + \nabla \cdot f(\nabla u^n). \]  
(5.2.25)

**Theorem 5.3.** For the semi-discrete scheme (5.2.25), we have the following results:

- (i) For the thin film model (5.1.5) with slope selection (5.1.8), if the constant \( \beta \) in (5.2.25) is sufficiently large, then (5.2.25) is unconditionally energy stable in the sense of \( E(u^{n+1}) \leq E(u^n) \), where the energy \( E \) is defined by (5.1.7);
• (ii) For the thin film model (5.1.5) without slope selection (5.1.9), if the constant $\beta$ in (5.2.25) satisfies $\beta \geq \frac{1}{2}$, then (5.2.25) is unconditionally energy stable in the sense of $E(u^{n+1}) \leq E(u^n)$, where the energy $E$ is defined by (5.1.7).

**Proof.** The proof of part (i) is similar to the proof of the last theorem and we will omit it here. For the thin film model (5.1.5) without slope selection (5.1.9), we observe that

$$||\partial_{\nabla u}^2 F(\nabla u)||_2 = \frac{1}{1 + |\nabla u|^2} \leq 1.$$ 

Note that

$$f(\nabla u) = \partial_{\nabla u} F(\nabla u) \quad \text{and} \quad \partial_{\nabla u} f(\nabla u) = \partial_{\nabla u}^2 F(\nabla u).$$

Consequently, for all $u$ we have

$$\max_{u \text{solves MBE}} ||\partial_{\nabla u} f(\nabla u)||_2 \leq 1. \quad \text{(5.2.26)}$$

Similar to (5.2.21), we obtain from (5.2.25) and (5.2.26) that

$$E(u^{n+1}) - E(u^n) \leq \frac{\epsilon^2}{2} \left(||\Delta u^{n+1}||_2^2 - ||\Delta u^n||_2^2 + (f(\nabla u^n), \nabla (u^{n+1} - u^n)) + \frac{1}{2}||\nabla (u^{n+1} - u(5))||_2^2 \right) \quad \text{(5.2.27)}$$

Taking $L^2$ inner product of (5.2.25) with $u^{n+1} - u^n$ yields

$$\frac{||u^{n+1} - u^n||_2^2}{k} = (-\epsilon^2 \Delta^2 u^{n+1} + \beta \Delta u^{n+1} - \beta \Delta u^n + \nabla \cdot f(\nabla u^n), u^{n+1} - u^n)$$

$$= -\epsilon^2(\Delta u^{n+1}, \Delta u^{n+1} - \Delta u^n) - \beta ||\nabla (u^{n+1} - u^n)||_2^2 - (f(\nabla u^n), \nabla (u^{n+1} - u^n))$$

$$= I_1 - \beta ||\nabla (u^{n+1} - u^n)||_2^2 - (f(\nabla u^n), \nabla (u^{n+1} - u^n)). \quad \text{(5.2.28)}$$

It can be shown that

$$I_1 = -\frac{\epsilon^2}{2} \left(||\Delta u^{n+1}||_2^2 - ||\Delta u^n||_2^2 + ||\Delta u^{n+1} - \Delta u^n||_2^2 \right). \quad \text{(5.2.29)}$$

Using (5.2.27)-(5.2.29) and the assumption $\beta \geq \frac{1}{2}$ yields

$$\frac{||u^{n+1} - u^n||_2^2}{k} \leq - \left(E(u^{n+1}) - E(u^n) + \frac{\epsilon^2}{2}||\nabla u^{n+1} - \nabla u^n||_2^2 \right),$$

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which leads to
\[ E(u^{n+1}) - E(u^n) \leq -\frac{\|u^{n+1} - u^n\|^2}{k} - \frac{\epsilon^2}{2} \|\nabla u^{n+1} - \nabla u^n\|^2 \leq 0. \] (5.2.30)

This proves the part (ii) of the theorem. \(\Box\)

In practical computations, for the Cahn-Hilliard equation and the MBE equation with slope selection, the assumption that \(\beta\) is sufficiently large can be relaxed. For example, take the double well potential \(F(u) = \frac{1}{4}(u^2 - 1)^2\) with \(|f'(u)| = |3u^2 - 1|\). As the physical solutions \(u\) is bounded in \([-1, 1]\), the condition (5.2.20) implies that \(\beta = 1\) is big enough for the stability. Similarly, for the MBE model with selection, \(\beta = 2\) will be sufficient for the stability. This is indeed confirmed by our numerical computations.

For the MBE equation without slope selection, the clean condition of \(\beta \geq \frac{1}{2}\) is due to the boundedness of (5.2.26). A similar observation of this nice property is also made and used in [77, 78].

### 5.3 SDC schemes and Semi-implicit SDC schemes

The spectral deferred correction was first introduced to solve the Cauchy problem for ODEs by Dutt et al. in [79]. The key idea of the SDC method is to convert the original ODEs into the corresponding Picard equation and then apply a deferred correction procedure in the integral formulation. The goal of SDC method is to achieve higher order accuracy schemes for both non-stiff and stiff problems. Below we will briefly describe the SDC method.

Consider the following ODE system:
\[ u'(t) = G(t, u(t)), \quad t \in (a, b], \]
\[ u(a) = u_a, \] (5.3.1)

where \(u(t), u_a \in R^n\) and \(G : [a, b] \times R^n \to R^n\). It is assumed that \(G\) is sufficiently smooth so that the discussion of higher order methods is appropriate.
The corresponding Picard integral equation to (5.3.1) is given below,

\[ u(t) = u_a + \int_a^t G(\tau, u(\tau))d\tau. \quad (5.3.2) \]

Given an initial approximation to the solution \( u^0(t) \), a residual function to measure the quality of the approximation is defined as follows,

\[ \epsilon(t, u^0) = u_a + \int_a^t G(\tau, u^0(\tau))d\tau - u^0(t). \quad (5.3.3) \]

By denoting the error function by \( \delta(t) = u(t) - u^0(t) \) and substituting \( u(t) = u^0(t) + \delta(t) \) into (5.3.2), we obtain

\[ \delta(t) = u_a + \int_a^t G(\tau, u^0(\tau) + \delta(\tau))d\tau - u^0(t). \quad (5.3.4) \]

Subtracting (5.3.3) from (5.3.4) gives

\[ \delta(t) = \int_a^t G(\tau, u^0(\tau) + \delta(\tau)) - G(\tau, u^0(\tau))d\tau + \epsilon(t). \quad (5.3.5) \]

Eq. (5.3.5) is referred to as the correction equation. After using some numerical method to discretize the correction equation (5.3.5), such as the explicit Euler method to non-stiff problems and the implicit Euler method to stiff problems, and adding the error function \( \delta(t) \) to the initial approximation \( u^0(t) \), we can get higher order approximated solution \( u^c(t) \), where \( u^c(t) = u^0(t) + \delta(t) \). In the following subsections, we present this procedure in more details.

### 5.3.1 SDC methods based on Euler methods

First we divide the computational time interval \([0, T]\) into \( N \) non-overlapping intervals \( 0 = t_0 < t_1 < \cdots < t_N = T \). We do the SDC procedure in every interval \([t_n, t_{n+1}]\).

Denoting the \( p + 1 \) Legendre-Guass-Radau IIa nodes (cf. [61]) on \([-1, 1]\) by \(-1 = r_0 < r_1 < \cdots < r_{p-1} < r_p = 1\) and letting

\[ \tau_i = \frac{t_{n+1} - t_n}{2} r_i + \frac{t_{n+1} + t_n}{2}, \quad i = 0, 1, \cdots, p, \]

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we obtain the spectral nodes on interval \([t_n, t_{n+1}]\) of the form \(t_n = \tau_0 < \tau_1 < \cdots < \tau_{p-1} < \tau_p = t_{n+1}\). Then the interval \([t_n, t_{n+1}]\) is divided into \(p\) subintervals, i.e. \([t_n, t_{n+1}] = \bigcup_{i=0}^{p-1} [\tau_i, \tau_{i+1}]\).

For convenience, we use the notation \(u_i = u(\tau_i)\) (similarly for \(\delta_i, \epsilon_i(u^0)\)) and \(\Delta \tau_i = \tau_{i+1} - \tau_i\), and take \(u_i^0\) to represent the initial approximation at \(\tau_i\) and \(u_i^c\) to represent the corrected approximation at \(\tau_i\). Once obtaining numerical approximations at these spectral nodes \(u_0^0, u_1^0, \cdots, u_p^0\) by stabilized semi-implicit schemes given in Section 2, we can then compute the corrections \(\delta_i\) to increase the accuracy for \(u^0\) by \(u_i^c = u_i^0 + \delta_i\).

One feasible way to discretize the correction equation (5.3.5) is the implicit Euler method as the phase-field models are usually stiff problems.

To be more specific, we set \(u_0^c = u_0^0\) and \(\delta_0 = 0\) as the initial value. Discretizing the correction equation (5.3.5) via the implicit Euler method, we have

\[
\delta_{i+1} = \delta_i + \Delta \tau_i [G(\tau_{i+1}, u_{i+1}^0 + \delta_{i+1}) - G(\tau_{i+1}, u_{i+1}^0)] + \epsilon_{i+1}(u^0) - \epsilon_i(u^0). \tag{5.3.6}
\]

Denote

\[
I_i^{i+1}(u^0) = \int_{\tau_i}^{\tau_{i+1}} G(s, u^0(s))ds, \tag{5.3.7}
\]

It follows from (5.3.3) that

\[
I_i^{i+1}(u^0) = \epsilon_{i+1}(u^0) - \epsilon_i(u^0) + u_{i+1}^0 - u_i^0. \tag{5.3.8}
\]

Note \(u_{i+1}^0 + \delta_{i+1} = u_{i+1}^c\). Substituting the above equation into (5.3.6) gives

\[
u_{i+1}^c = u_i^c + \Delta \tau_i [G(\tau_{i+1}, u_{i+1}^c) - G(\tau_{i+1}, u_{i+1}^0)] + I_i^{i+1}(u^0), \tag{5.3.9}
\]

which gives an implicit equation for \(u^c\). The remaining is to compute the integral (5.3.7) using the discrete values at the spectral nodes. One way is to approximate the continuous function \(G(s, u^0)\) by using the Lagrange interpolation polynomials:

\[
G_p(s, u^0) = \sum_{j=0}^{p} G(\tau_j, u_j^0) L_j^p(s), \tag{5.3.10}
\]
where $L_p^p(s)$ is the Lagrange basis polynomial of degree $p$ associate with the spectral points $\{\tau_j\}_{j=0}^p$. Approximate $I_i^{i+1}(u^0)$ by

$$I_i^{i+1}(u^0) \approx \int_{\tau_i}^{\tau_{i+1}} G_p(s, u^0(s))ds = \sum_{j=0}^{p} G(\tau_j, u^0_j)c^p_{ij}, \quad (5.3.11)$$

where

$$c^p_{ij} = \int_{\tau_i}^{\tau_{i+1}} L^p_j(s)ds. \quad (5.3.12)$$

If the correction procedure is implemented $k$ times, we can enhance the order of accuracy for the approximation $u^0$ by $\min\{k, 2p\}$ if $p+1$ Gauss-Radau nodes (including the two endpoints) are used, (cf. [79, 81]).

### 5.3.2 Semi-implicit SDC Methods

As the governing equations for phase-field models involving very small parameters, the resulting discretized equations may be very stiff. As a result, the explicit Euler method is not appropriate for the sake of stability requirement. However, the conventional implicit Euler method leads to a nonlinear system, which affects the numerical efficiency. This motivates us to use the semi-implicit SDC methods [93].

Similar to the last subsection, we drive the semi-implicit SDC for the correction equation (5.3.5) as

$$u^c_{i+1} = u^c_i + \Delta \tau_i [G_I(\tau_{i+1}, u^c_{i+1}) - G_I(\tau_{i+1}, u^0_{i+1}) + G_E(\tau_i, u^c_i) - G_E(\tau_i, u^0_i)] + I_i^{i+1}(u^0). \quad (5.3.13)$$

Below we just take the Cahn-Hilliard equation as an example to illustrate how to implement SDC to the phase-field models. To eliminate the ambiguity of notation, we denote time step $\Delta \tau_i = k$ in (5.2.18) and also let

$$G_I(s, u(s)) = -\epsilon^2 \Delta^2 u + \beta \Delta u$$

and

$$G_E(s, u(s)) = -\beta \Delta u + \Delta f(u).$$
Then we get

\[
uc_{i+1} = uc_i + k\bigg((−\epsilon^2 \Delta^2 + \beta \Delta)uc_{i+1} - (−\epsilon^2 \Delta^2 + \beta \Delta)uc_0_{i+1} \\
+ (−\beta \Delta uc_i + \Delta f(uc_i)) - (−\beta \Delta uc_0_i + \Delta f(uc_0_i))\bigg) + I_{i}^{i+1}(u^0),
\]

which is given by scheme (5.2.18). To solve (5.3.14) for \(uc\), we only need to solve a linear system as the implicit term \(F_I = F_c\) is linear. The key factor for solving the linear system efficiently is to handle the Laplace operators involved, which will be discussed in the next section.

We close this section by reviewing some convergence issues of the SDC method. We mention that the convergence for the SDC method on uniform quadrature nodes with high-order RK correction steps was established in [80] using a smoothness of rescaled error vector approach. With the same number of function evaluations, it was shown in [80] that the use of the higher-order integrators can have one magnitude of accuracy improvement. However, the order increment in the correction loop does not hold for non-uniform grids, e.g., the Gaussian quadrature nodes are excluded. In [81], a general framework for the convergence of the SDC method was established, which can recover high-order rate of convergence with non-uniform quadrature nodes. These theoretical results show that the SDC method is not only an efficient numerical strategy, but also with a rigorous theoretical justification.

5.4 Spatial discretization and a fast solver

After discretizing governing equations in time as described in Section 2, we end up with a general form of partial differential equations as follows,

\[
u = −\gamma \Delta^2 u + \theta \Delta u + b,
\]

where \(\gamma\) and \(\theta\) are non-negative constant parameters (\(\gamma = 0\) is for the Allen-Cahn equation) and \(b\) is the given source term. Below we will use the central finite difference to discretize the Laplace operator.
Without loss of generality, we consider a computing domain $[0, 1] \times [0, 1]$ with mesh grid $\Delta x = \Delta y = h = \frac{1}{N}$. To simplify notations, let $u_{j,k} = u(x_j, y_k)$ and use $U = [u_{jk}]_{j=1,\cdots,N}^{k=1,\cdots,N}$ to represent the matrix of unknowns. The central difference scheme to approximate the Laplace operator is given below

$$
\Delta u_{j,k} \approx \frac{u_{j-1,k} - 2u_{j,k} + u_{j+1,k}}{h^2} + \frac{u_{j,k-1} - 2u_{j,k} + u_{j,k+1}}{h^2} + O(h^2).
$$

(5.4.2)

By letting

$$
M = \frac{1}{h^2} \begin{bmatrix}
-2 & 1 & 0 & \cdots & 0 & 1 \\
1 & -2 & 1 & 0 & \cdots & 0 \\
0 & 1 & -2 & 1 & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & 1 & -2 & 1 \\
1 & 0 & \cdots & 0 & 1 & -2
\end{bmatrix},
$$

we can obtain from (5.4.2) the matrix form

$$
\Delta U \approx UM + MU + O(h^2).
$$

(5.4.3)

Note that the matrix $M$ is not strict tridiagonal as the top right and the lower left values are nonzero which is due to the periodic boundary conditions. The matrix $M$ is strict tridiagonal if the homogeneous Dirichlet boundary conditions are given. Similarly, we can get the matrix form for the biharmonic Laplace operator:

$$
\Delta^2 U = \Delta(\Delta U) \approx (\Delta U)M + M(\Delta U) + O(h^2)
$$

$$
= M^2U + 2MU + UM^2 + O(h^2).
$$

(5.4.4)

As $M$ is a circulant matrix, it can be diagonalized by utilizing the unitary discrete Fourier transform matrix $V_N$ (see, e.g. [82]):

$$
V_N = \frac{1}{\sqrt{N}} F_N, \text{ where } F_N = (f_{jk}) \text{ with } f_{jk} = e^{-2jk\pi i/N}, \text{ for } 0 \leq j, k < N.
$$

In fact, we have

$$
M = V_N^* \Lambda V_N, \text{ where } \Lambda = \text{diag}(F_N \cdot c) = (\lambda_1, \cdots, \lambda_N)^T \text{ and } c \text{ is the first column of } M.
$$
Substituting the above diagonalized matrix into (5.4.3) and (5.4.4) and using the fact $V_N^*V_N = I_N$ yield
\[
\Delta U \approx UV_N^*AV_N + V_N^*AV_NU + O(h^2), \\
\Delta^2 U \approx V_N^*A^2V_NU + 2V_N^*AV_NUV_N^*AV_N + UV_N^*A^2V_N + O(h^2).
\]

Consequently, we obtain the discrete form for (5.4.1) with second-order accuracy:
\[
U = \left(-\gamma(V_N^*A^2V_NU + 2V_N^*AV_NUV_N^*AV_N + UV_N^*A^2V_N)
\right)
\]
\[
+ \theta(UV_N^*AV_N + V_N^*AV_NU) + B,
\]
where $B$ is the discrete matrix form of $b$. By defining $\bar{U} = V_NUV_N^*$ and $\bar{B} = V_NBV_N^*$ and multiplying $V_N$ and $V_N^*$ to the left-hand side and the right-hand side of (5.4.7) respectively, we further simplify the equation as
\[
\bar{U} + \gamma(\Lambda^2\bar{U} + 2\Lambda\bar{U}\Lambda + \bar{U}\Lambda^2) - \theta(\Lambda\bar{U} + \bar{U}\Lambda) = \bar{B}.
\]
Denote the left-hand side of (5.4.8) as $G(\bar{U})$. Since $\Lambda$ is a diagonal matrix with entries $\lambda_j$, it can be verified that
\[
g_{j,k} = (1 + \gamma(\lambda_j + \lambda_k)^2 - \theta(\lambda_j + \lambda_k))\bar{u}_{j,k} \Rightarrow \bar{u}_{j,k} = \frac{\bar{b}_{j,k}}{g_{j,k}}.
\]
Once $\bar{U}$ is obtained, it is easy to compute $U = V_N^*\bar{U}V_N$.

Note that the size of the stiff matrix $M$ for the Laplace operator is $N \times N$ instead of sparse $N^2 \times N^2$ matrixes in the usual cases. As the eigenvalues $\lambda_i$ can be prepared beforehand, the above computation can be made very efficient. Moreover, only the values $U^k$ at $p$ levels require to be stored, with $2p \times N^2$ in total.

### 5.5 Efficiency enhancement with $p$-adaptivity

The time-discretization using the stabilized semi-implicit schemes with the SDC scheme seems perfectly suitable for simulating the three phase-field models as it is of high order and is energy stable. Unfortunately, numerical instability is observed
in large time numerical simulations, as demonstrated in Fig. 5.4. The reason for the instability may be caused by the large number of corrections used. Without using correction, the energy stability can be preserved but accuracy may not be satisfactory. However, using too many corrections may cause the above mentioned blow-up. It remains to balance the accuracy and stability. To this end, we will propose an adaptive strategy to adjust the correction number. Inspired by the idea in [58], we give a monitor function to predict the correction number at $(n + 1)^{th}$ step using the discrete energies $E_h(u^n)$ and $E_h(u^{n-1})$:

$$N_p = \min\{N_{max}, \max\{0, N_{max} + \text{fix}[\log_\eta(|E_h(u^n) - E_h(u^{n-1})| + \eta^{-(N_{max}+1)})]\}\},$$

(5.5.1)

where $\eta$ is a positive constant, $N_{max}$ is the maximum number of corrections and $\text{fix}[\cdot]$ represents the integer part of a number. Below we will explain the motivation of using (5.5.1) to predict $N_p$. It is clear that more corrections are needed in the region where the energy decays fast. In other words, if the dynamical process evolves dramatically then more corrections are required to capture the dynamical evolution correctly. More specifically, the relationship between $N_p$ and the energy change is given as following:

$$N_p = \begin{cases} 
0, & \text{if } |E_h(u^n) - E_h(u^{n-1})| < \eta^{-N_{max}} \\
k, & \text{if } \eta^{-N_{max}+k} \leq |E_h(u^n) - E_h(u^{n-1})| < \eta^{-N_{max}+k+1} \\
N_{max}, & \text{if } |E_h(u^n) - E_h(u^{n-1})| \geq \eta^{-1}
\end{cases},$$

(5.5.2)

where $N_{max}$ is upper bounded by $2p - 1$ as the accuracy order of the interpolation on the $p + 1$ Gauss-Radau nodes is $2p$ and the parameter $\eta$ can be fixed as 3 or 5 in the later numerical tests.

Note that the physical energy decreasing property motivates us to use the energy difference at $t_{n-1}$ and $t_n$ for choosing the number of corrections. Firstly, as observed from the energy curves in Fig. 5.1, the energy variation in most time regimes is very small, so $N_p = 0$ should be chosen in most of the time intervals. This implies that
Figure 5.4: Example 5.1: Blowing up phenomenon for the SDC method with uniform number of corrections for long time simulation.

only first order SDC method is used, which guarantees the energy stability in general. Secondly, in the transition regime, the energy variation is between $\eta^{-N_{\text{max}}}$ and $\eta^{-1}$, which indicates some variable value of $Np$ is used based on the size of the energy variation. Thirdly, if the energy variation exceeds $\eta^{-1}$, then the maximum number of correction should be used. In the later two cases, the energy decreasing property may not be preserved locally. However, as the total number of the intervals relevant to the last two cases is very small, it is expected that the overall energy stability can be preserved well. In other words, the choice of (5.5.2) seems very useful to balance the accuracy and overall energy stability.
5.6 Numerical experiments

5.6.1 Convergence tests

Example 5.1. We first test the convergence orders. To this end, consider the numerical solutions of two-dimensional Allen-Cahn equation with \( f(u) = u^3 - u \) and \( \epsilon^2 = 0.01 \). To verify the convergence order, we add a source term to the ACE such that the exact solution is

\[
u(x, y) = \exp(-2t) \sin x \sin y, \quad (x, y) \in [0, 2\pi] \times [0, 2\pi].\]

We use the fast numerical solver proposed in the previous section for the spatial discretization and the semi-implicit spectral deferred correction method for the time discretization. To test the numerical accuracy, we take a spatial grid of 600×600 with a coarse time step \( \tau = 0.4 \). The \( L^2 \)-norm error and \( L^\infty \)-norm error at \( T = 4 \) with \( p = 4 \), \( \beta = 1 \) and \( Np = 1, 2, 3, 4 \) respectively are shown in Table 5.1. It is observed that the numerical scheme with constant \( Np \) corrections in all time intervals gives optimal-order of accuracy in time.

5.6.2 SDC allows large time step

The following two examples are designed to study whether large time steps are suitable for phase-field simulations.

Example 5.2. We will use the numerical example given in [57], i.e., we consider the Cahn-Hilliard equation with \( f(u) = u^3 - u \) and \( \epsilon^2 = 0.01 \) with the initial condition

\[
u_0(x, y) = 0.05 \sin x \sin y, \quad 0 \leq x, y \leq 2\pi\]

and the periodic boundary condition.

We take the numerical solutions on a 400×400 mesh and the uniform time step \( dt = 0.001 \) as the “reference” solution. We fix \( p = 4 \), \( \beta = 1 \) and change \( Np = 0, 1, 2, 4 \).
<table>
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<th>( Np )</th>
<th>( | u_{h,\tau} - u |_2 )</th>
<th>( \tau = 0.4 )</th>
<th>( \tau/2 )</th>
<th>( \tau/4 )</th>
<th>( | u_{h,\tau} - u |_\infty )</th>
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<td>2.42</td>
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<td>5.46e-1</td>
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<tr>
<td></td>
<td>( | u_{h,\tau} - u |_\infty )</td>
<td>5.46e-1</td>
<td>1.85e-01</td>
<td>4.97e-2</td>
<td></td>
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<tr>
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<td>8.87e-3</td>
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<tr>
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<td>( | u_{h,\tau} - u |_\infty )</td>
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<td></td>
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<td></td>
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</tr>
</tbody>
</table>

Table 5.1: Example 5.1: Numerical errors and convergent rates against the number of corrections in the SDC method for the 2D Allen-Cahn equation at \( T = 4 \).
Figure 5.5: Example 5.2: Energy evolutions with different time steps and different numbers of corrections for the Cahn-Hilliard equation.

to implement the SDC methods. The energy evolution from $T = 0$ to 7 with different number of corrections are presented in Fig. 5.5, where it is observed that the energy curves converge to the reference solution as the number of corrections increased even with a quite large time step 1/20. When $Np = 4$, the energy curve almost coincides with the reference solution. In Fig. 5.6, numerical solutions at $T = 2$ are obtained with $dt = 1/4$. It is well observed that the coarse stepsize together with 4 or 5 corrections can significantly improve the quality of the approximation.

**Example 5.3.** This example uses large time steps to simulate the thin film model without slope selection. We take the same initial condition, boundary condition, physical parameters as in Example 5.2.

We use the same computational grids both in time and in space as in Example 2 but the parameter $\beta$ in the numerical scheme (5.2.25) is chosen to be 0.5. Convergence with respect to the number of corrections is shown in Fig. 5.7.
Figure 5.6: Example 5.2: Numerical solutions for the Cahn-Hilliard equation at time $T = 2$ using the SDC method.

5.6.3 Long time simulations

It is observed from Figs. 5.5-5.7 that large time steps with some corrections can indeed improve the solution accuracy and also capture the dynamical solution correctly. However, as demonstrated in Fig. 5.3, the balance of accuracy and energy stability does not hold for larger $T$. This requires the use of an adaptive approach.
Figure 5.7: Example 5.3: Numerical solutions of the thin film model without slope selection at time $T = 2$ using different number iterations. It is seen with 5 iterations, $dt = 0.25$ gives almost the same results as the $dt = 10^{-3}$ results.

Example 5.4. We will use the adaptive the SDC scheme for long time simulation of the Cahn-Hilliard equation with initial condition

$$u_0(x, y) = 0.05 \sin x \sin y + 0.001, \quad 0 \leq x, y \leq 2\pi,$$

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Figure 5.8: Example 5.4: Energy curves of the Cahn-Hilliard equation by different schemes with different time steps.

and the periodic boundary condition. The parameter \( \epsilon^2 \) is chosen as 0.01.

The mesh grid in space is fixed as 400 \( \times \) 400. We take the numerical solutions with small uniform time step \( dt = 0.001 \) as the “reference” solution. We take \( p = 4 \) in the SDC method, and \( \beta = 1 \) in (5.2.18), \( \eta = 5 \), \( N_{max} = 5 \) in (5.5.2) and set \( N_p = N_{max} \) at the first step. Then we use the monitor function to update \( N_p \) afterwards. The energy curves and the numerical results are showed in Figs. 5.8-5.11.

In Fig. 5.8, with the adaptive SDC scheme we can use \( dt = 0.04 \) to obtain nearly coincident energy curve as that for \( dt = 0.001 \) without adaptivity. On the other hand, the energy curve will be far from the reference energy curve if we use \( dt = 0.04 \) without adaptivity, especially before \( T = 10 \), which can be seen in the locally magnified energy curves from \( T = 2 \) to 8. The number of iterations used in each time step is plotted in Fig. 5.9, where as expected larger slope of the energy curve corresponds to bigger number of corrections. The CPU time comparison is presented in Fig. 5.10, where it is seen that our adaptive SDC scheme consumes more CPU time at beginning as more corrections are needed to capture the fast
Figure 5.9: Example 5.4: Energy curves of the Cahn-Hilliard equation (left \(y\)-axis) and number of corrections (right \(y\)-axis) by the adaptive SDC schemes.

Figure 5.10: Example 5.4: CPU time comparison between different schemes for the Cahn-Hilliard equation.
dynamical evolution. However, our adaptive SDC scheme can enhance the efficiency significantly in the long time computation. The numerical solutions at different time levels are presented in Fig. 5.11, where it is observed that the solution dynamics can be captured correctly with larger time steps when adaptive strategy is employed.

Figure 5.11: Example 5.4: Solutions at different time, using (a) direct stabilized semi-implicit schemes without SDC and $dt = 0.001$; (b) stabilized semi-implicit schemes without SDC and $dt = 0.04$; and (c) adaptive SDC scheme with $dt = 0.04$.

**Example 5.5.** Consider the thin film model with slope selection with $f(\nabla u) = (1 - |\nabla u|^2)\nabla u$ with the initial value

$$u_0 = 0.1(\sin 3x \sin 2y + \sin 5x \sin 5y)$$

and the periodic boundary condition. The parameter $\epsilon^2$ is 0.1 and the computation domain is $\Omega = [0, 2\pi] \times [0, 2\pi]$.

The spatial space is divided into a $400 \times 400$ mesh. We fix $p = 3$, $\beta = 2$ and set $\eta = 3$ and $Np = 5$ at first time step. We take the numerical result by the stabilized
semi-implicit schemes without SDC with time step $dt = 0.001$ as the “reference” solution. The energy evolutions and the number of corrections are shown in Figs. 5.12 and 5.13, respectively. We can see from Fig. 5.12 that the energy curve obtained by the adaptive SDC scheme with $dt = 0.02$ is in good agreement with the reference curve, while the difference between the $dt = 0.001$ and $dt = 0.02$ curves, both without adaptivity, is very big. It is also observed from Fig. 5.13 that the number of corrections is proportional to the slope of the energy curve. In Fig. 5.14, the CPU time comparison is made, where it is clearly seen that the adaptive computation can indeed enhance the efficiency.

Figure 5.12: Example 5.5: Energy curves of the thin film with slope selection by different schemes with different time steps.

Example 5.6. Consider the thin film model without slope selection with $f(\nabla u) = -\frac{\nabla u}{1 + |\nabla u|^2}$ as given in [36] with the same initial values as Example 5.5.

We fix $\beta = 0.5$ and $\eta = 5$ and set the same values as Example 5 for other parameters at first time step. Similarly we obtain satisfactory numerical results as plotted in Figs. 5.15 and 5.16, and the CPU time improvement as plotted in Fig. 5.17. To test the robustness of the parameters, we also tried $\eta = 2$ and $\eta = 7$ in
the above two examples. In both cases, the corresponding numerical results are also satisfactory.

Figure 5.13: Example 5.5: Energy curves of the thin film model with slope selection (left $y$-axis) and number of corrections (right $y$-axis) by the adaptive SDC schemes.

Figure 5.14: Example 5.5: CPU time comparison between different schemes for the thin film model with slope selection.
Figure 5.15: Example 5.6: Energy curves of the thin film without slope selection by different schemes with different time steps.

Figure 5.16: Example 5.6: Energy curves of the thin film model without slope selection (left y-axis) and number of corrections (right y-axis) by the adaptive SDC schemes.

5.7 Concluding remarks

In this paper, a temporal $p$-adaptive scheme based on stabilized semi-implicit schemes is designed for solving the phase field models. The $p$-adaptivity is realized by employ-
Figure 5.17: Example 5.6: CPU time comparison between different schemes for the thin film model without slope selection.

Implementing the spectral deferred correction method at some needed time levels. In space, we first use a fast solver for the Laplace operator and then use DFT matrix technique to diagonalize the resulting circulant linear system. This approach highly enhances the overall solution efficiency.

We aim to balance the accuracy and stability by using the $p$-adaptive scheme. To this end, a practical strategy is proposed to control the number of the corrections based on the variation of the energy curve. This turns out to be a simple and effective approach.

Numerical experiments demonstrate that the proposed $p$-adaptive scheme is very effective for solving the phase-field models. It can enhance accuracy of the numerical solution by increasing the number of corrections to capture the fast time scale dynamics and also save computational time by using lower order method for slow dynamics. With $p$-adaptive technique, quite larger time steps (e.g., $dt=1/25$) can be used to catch both solution dynamics and steady states.
Chapter 6

Summary and future work

6.1 Summary of the thesis

During my PhD period, I am devoted to developing accurate, efficient and robust numerical methods and the related numerical analysis for three representative phase-field models, namely the Allen-Cahn equation, the Cahn-Hilliard equation and the thin film model. The numerical stability analysis is the core of this thesis. We investigate several numerical schemes from three different aspects of numerical stability, that is, nonlinear energy stability, numerical maximum principle and uniform $L^2$-stability.

For the energy stability, we have studied stabilized Crank-Nicolson/Adams-Bashforth schemes for both Allen-Cahn equations and Cahn-Hilliard equations. It is shown that the proposed time discretization schemes are either unconditionally energy stable or conditionally energy stable under some reasonable stability conditions. We also applied the multi-step implicit-explicit methods to approximate the Allen-Cahn equation, and we have investigated the relationship between the parameters and the nonlinear energy stability for the first-order and second-order schemes.

We have established numerical maximum principle for several kinds of Allen-Cahn-type equations: the simple Allen-Cahn equation with constant mobility and polynomial free energy, the generalized Allen-Cahn equation with nonlinear degenerate mobility and logarithmic free energy as well as added advection term and fractional-in-space Allen-Cahn equations. Point-wise error estimates are given for the first two equations, which is nontrivial if without numerical maximum principle.
Besides the first-order semi-implicit scheme, we have proved that the second-order Crank-Nicolson scheme can also preserve the numerical maximum principle for the last equation, which obviously holds for the other two models.

Furthermore, we achieve the spectral convergence rate by Fourier spectral methods for the Allen-Cahn equation. This is based on a priori stability: $L^2$-stability which is a novel stability for the Allen-Cahn equation. We first prove that the continuous Allen-Cahn equation satisfies $L^p$-stability. However, for both Fourier Galerkin methods and Fourier collocation methods, we can only recover the $L^2$-stability.

Besides the numerical stability analysis, we also focus on the long time simulations of these phase-field models. We develop a high-order and energy stable scheme to simulate these three phase-field models by combining the semi-implicit spectral deferred correction method and first-order semi-linear schemes with stabilized term. It is found that the accuracy improvement may affect the overall energy stability. To compromise the accuracy and stability, a local $p$-adaptive strategy is proposed to enhance the accuracy by sacrificing some local energy stability in an acceptable level. Numerical results demonstrate the high effectiveness of our proposed numerical strategy.

6.2 Future research

Part of my future work is based on and as a continuation of current work. Considering the Allen-Cahn, Cahn-Hilliard equations and thin film models, I am planning to take the following problems into consideration:

1. Seek high order numerical schemes either in time or in space to preserve the maximum principle for the Allen-Cahn equation. The most desired result is a three-level scheme to fulfil all the requirements mentioned above, since our current results are all built on two-level schemes. Once done, I believe Runge-Kutta methods can be used to achieve higher-order schemes.
2. Achieve more elegant error estimates. This may be done particularly as we can control numerical solutions uniformly bounded by 1 pointwisely.

3. Try to get a more accurate $L^\infty$ estimate for the spectral methods based on the uniform $L^2$-stability since most results in our numerical experiments satisfy the maximum principle quite well.

4. Design efficient numerical methods for the Cahn-Hilliard equation with logarithmic free energy to keep solutions strictly in $(-1, 1)$. The key difficulty is due to the loss of the maximum principle for the biharmonic operator. One possible way is to approximate the Cahn-Hilliard equation by using the corresponding viscous Cahn-Hilliard equation with logarithmic free energy and try to convert the viscous Cahn-Hilliard equation into the Allen-Cahn equation. However, this task seems very challenging and it requires some elegant tools and analysis techniques.

Moreover, applying our results to Allen-Cahn or Cahn-Hilliard Navier-Stokes system is also a meaningful work, which are used to model two-phase flows recent years. Besides these, during my PhD period, I have learnt a number of other topics in computational mathematics, such as adaptive moving mesh methods, conservation laws, image processing, spectral methods, artificial boundary conditions, Maxwell equations, etc. I will be happy to do some further research in these fields once I have the opportunity.
Bibliography


Curriculum Vitae

Academic qualifications of the thesis author, Mr. YANG Jiang:

- Received the degree of Bachelor of Mathematics and Applied Mathematics from Zhejiang University, June 2010.

Journal Publications


Submitted Papers


Preprint/ Preparing Works


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