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VARIABLE STEP-SIZE BDF3 METHOD FOR ALLEN-CAHN EQUATION*

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Abstract

In this work, we analyze the three-step backward differentiation formula (BDF3) method for solving the Allen-Cahn equation on variable grids. For BDF2 method, the discrete orthogonal convolution (DOC) kernels are positive, the stability and convergence analysis are well established in [Liao and Zhang, Math. Comp., 90 (2021), 1207–1226] and [Chen, Yu, and Zhang, arXiv:2108.02910, 2021]. However, the numerical analysis for BDF3 method with variable steps seems to be highly nontrivial due to the additional degrees of freedom and the non-positivity of DOC kernels. By developing a novel spectral norm inequality, the unconditional stability and convergence are rigorously proved under the updated step ratio restriction $r_k := \tau_k/\tau_{k-1} \leq 1.405$ for BDF3 method. Finally, numerical experiments are performed to illustrate the theoretical results. To the best of our knowledge, this is the first theoretical analysis of variable steps BDF3 method for the Allen-Cahn equation.

Mathematics subject classification: 65L06, 65M12.
Key words: Variable step-size BDF3 method, Allen-Cahn equation, Spectral norm inequality, Stability and convergence analysis.

1. Introduction

The objective of this paper is to present a rigorous stability and convergence analysis of the BDF3 method with variable steps for solving the Allen-Cahn equation [2]

$$\begin{cases} \partial_t u - \varepsilon^2 \Delta u + f(u) = 0, & (x,t) \in \Omega \times (0,T], \\ u(0) = u_0, \end{cases} \tag{1.1}$$

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where the nonlinear bulk force is given by $f(u) = F'(u) = u^3 - u$, and the parameter $\varepsilon > 0$ represents the interface width. For simplicity, we consider the periodic boundary conditions. The above Allen-Cahn equation can be viewed as an L^2-gradient flow of the following free energy functional:

$$E[u] = \int_\Omega \left(\frac{\varepsilon^2}{2}|\nabla u|^2 + F(u)\right) dx, \quad F(u) = \frac{1}{4}(u^2 - 1)^2. \tag{1.2}$$

In other words, the Allen-Cahn equation (1.1) admits the energy dissipation law

$$\frac{dE[u]}{dt} = -\int_\Omega |\partial_t u|^2 dx \leq 0. \tag{1.3}$$

Let $N \in \mathbb{N}$ and choose the nonuniform time levels $0 = t_0 < t_1 < \cdots < t_N = T$ with the time-step $\tau_k = t_k - t_{k-1}$ for $1 \leq k \leq N$. For any time sequence $\{v^n\}_{n=0}^N$, denote

$$\nabla_\tau v^n := v^n - v^{n-1}, \quad \partial_\tau v^n := \frac{\nabla_\tau v^n}{\tau_n}, \quad n \geq 1.$$

For $k = 1, 2, 3$, let $\Pi_{n,k} v$ denote the Lagrange interpolating polynomial of a function v over $k+1$ nodes $t_n, t_{n-1}, \ldots, t_{n-k}$. Define the adjacent time step ratio

$$r_k := \frac{\tau_k}{\tau_{k-1}}, \quad k \geq 2.$$

Let $v^n = v(t_n)$. The BDF3 scheme is defined by [5,13,15,16,21,23]

$$\begin{aligned} D_3 v^n = (\Pi_{n,3} v)'(t_n) &= b_0^{(n)} \nabla_\tau v^n + b_1^{(n)} \nabla_\tau v^{n-1} + b_2^{(n)} \nabla_\tau v^{n-2} \\ &= \sum_{k=1}^n b_{n-k}^{(n)} \nabla_\tau v^k, \quad n \geq 3, \end{aligned} \tag{1.4}$$

where

$$\begin{aligned} b_0^{(n)} &= \frac{(1 + r_{n-1})\left[1 + 2r_n + r_{n-1}\left(1 + 4r_n + 3r_n^2\right)\right]}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\ b_1^{(n)} &= -\frac{r_n^2[(1 + 2r_{n-1} + r_n r_{n-1})^2 - r_{n-1}(1 + r_{n-1})]}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\ b_2^{(n)} &= \frac{r_n^2 r_{n-1}^3 (1 + r_n)^2}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \quad b_j^{(n)} = 0, \quad j \geq 3. \end{aligned} \tag{1.5}$$

Since BDF3 scheme needs three starting values, for concreteness, we use BDF1 and BDF2 schemes to respectively compute the first-level solution u^1 and second-level solution u^2, namely,

$$D_3 v^1 := D_1 v^1 = \frac{\nabla_\tau v^1}{\tau_1}, \quad D_3 v^2 := D_2 v^2 = \frac{1 + 2r_2}{\tau_2(1 + r_2)} \nabla_\tau v^2 - \frac{r_2^2}{\tau_2(1 + r_2)} \nabla_\tau v^1. \tag{1.6}$$

We recursively define a sequence of approximations u^n to the nodal values $u(t_n)$ of the exact solution by BDF3 method

$$D_3 u^n - \varepsilon^2 \Delta u^n + f(u^n) = 0, \quad n \geq 1, \tag{1.7}$$

where the initial data $u^0 = u_0$ and $f(u^n) = (u^n)^3 - u^n$.

The BDF3 operator (1.4) and (1.6) are regarded as a discrete convolution summation

$$D_3 v^n = \sum_{k=1}^{n} b_{n-k}^{(n)} \nabla_\tau v^k, \quad n \geq 1, \tag{1.8}$$

where

$$b_0^{(1)} = \frac{1}{\tau_1}, \quad b_0^{(2)} = \frac{1+2r_2}{\tau_2(1+r_2)}, \quad b_1^{(2)} = -\frac{r_2^2}{\tau_2(1+r_2)}$$

in (1.6) and $b_{n-k}^{(n)}$ in (1.5).

Following the approach of [7, 18], the discrete orthogonal convolution (DOC) kernels are defined by

$$d_0^{(n)} := \frac{1}{b_0^{(n)}}, \quad d_{n-k}^{(n)} := -\frac{1}{b_0^{(k)}} \sum_{j=k+1}^{n} d_{n-j}^{(n)} b_{j-k}^{(j)}, \quad 1 \leq k \leq n-1. \tag{1.9}$$

Moreover, the DOC kernels $\{d_{n-k}^{(n)}\}_{k=1}^n$ satisfy the discrete orthogonal identity

$$\sum_{j=k}^{n} d_{n-j}^{(n)} b_{j-k}^{(j)} \equiv \delta_{nk}, \quad 1 \leq k \leq n. \tag{1.10}$$

For convenience, we introduce the following matrices:

$$B := \begin{pmatrix} b_0^{(1)} & & & & \\ b_1^{(2)} & b_0^{(2)} & & & \\ b_2^{(3)} & b_1^{(3)} & b_0^{(3)} & & \\ & \ddots & \ddots & \ddots & \\ & & b_2^{(n)} & b_1^{(n)} & b_0^{(n)} \end{pmatrix}, \quad D := \begin{pmatrix} d_0^{(1)} & & & & \\ d_1^{(2)} & d_0^{(2)} & & & \\ d_2^{(3)} & d_1^{(3)} & d_0^{(3)} & & \\ \vdots & \vdots & \ddots & \ddots & \\ d_{n-1}^{(n)} & d_{n-2}^{(n)} & \cdots & d_1^{(n)} & d_0^{(n)} \end{pmatrix}, \tag{1.11}$$

where the discrete convolution kernels $b_{n-k}^{(n)}$ and the DOC kernels $d_{n-k}^{(n)}$ are defined in (1.8) and (1.9), respectively. From the discrete orthogonal identity (1.10), there exists $D = B^{-1}$.

The variable time-stepping technique is powerful in capturing the multi-scale behaviors (e.g. the solution changes rapidly in certain regions of time) of phase fields model including the Allen-Cahn model. Due to the strong stability (A-stable), the numerical analysis of variable steps BDF2 method for ODEs and PDEs receives much attentions including some early works [3, 9, 10, 22] and very recent works [7, 8, 16, 18]. However, the numerical analysis for BDF3 method with variable steps seems to be highly nontrivial (compared with the BDF2 method). As for variable steps BDF3 method for ODEs, Grigorieff *et al.* proved that it is zero-stable if the adjacent time-step ratio $r_k < 1.08$ [12] and improved to $r_k < 1.292$ [13], $r_k < 1.462$ [4]. Based on a spectral radius approach, Guglielmi and Zennaro proved the zero-stability of variable steps BDF3 method for $r_k < 1.501$ [14]. Variable steps implicit-explicit BDF3 method is presented by Wang and Ruuth [23], where the zero-stability with $r_k < 1.501$ is also proved for ODEs. Recently, the stability is established under the adjacent time-step ratio $r_k < 2.553$ of variable steps BDF3 method for ODE problem [15]. The stability of the variable steps BDF3 method for a parabolic problem is derived by Calvo and Grigorieff [5] under the time-step ratio $r_k \leq 1.199$. However, it contains a factor $\exp(C\Gamma_n)$ with $\Gamma_n = \sum_{k=2}^n |r_k - r_{k-1}|$, the quantity Γ_n may be unbounded at vanishing step sizes for certain choices of time-steps. We are unaware of any other published works on the stability analysis of the variable steps BDF3 method for a time-dependent PDEs. After we submitted this work, we became aware of recent work on variable-step BDF3 time-stepping for diffusion equations under the ratio $r_k \leq 1.487$ [17]. In this paper, the variable steps BDF3 scheme is investigated to solve the Allen-Cahn equation. For the BDF2 method, the associated DOC kernels are positive, the stability and convergence analysis are well established [7, 18]. However, the DOC kernels are not always positive and the additional degrees of freedom are involved for BDF3 method, which implies the numerical analysis seems to be highly nontrivial. By developing a novel spectral norm inequality, the unconditional stability and convergence are rigorously proved under the updated step ratio restriction $r_k \leq 1.405$ for BDF3 method. As far as we know, this is the first theoretical analysis of variable steps BDF3 method for the Allen-Cahn equation.

The rest of this paper is organized as follows. In Section 2, we show that the upper bound of the fixed adjacent time-step ratio is less than $\sqrt{3}$ in a sense of the positive semi-definiteness of the matrix B in (1.11). In Section 3, we prove the variable adjacent time-step ratio $r_k \leq 1.405$, which plays an important role in our numerical analysis. In Section 4, the unique solvability of the variable-steps BDF3 scheme (1.7) is established in Theorem 4.1. A discrete energy stability is proved under the adjacent time-step ratio $r_k < 1.405$ in Theorem 4.2. By developing a novel spectral norm inequality in Lemma 5.2, the unconditional stability and the convergence of BDF3 scheme (1.7) are rigorously proved in Section 5. Finally, numerical experiments are carried out to corroborate the theoretical results.

2. Estimate for Fixed Adjacent Time-Step Ratio

In this section, we show that the upper bound of fixed adjacent time-step ratio is less than $\sqrt{3}$ in a sense of the positive semi-definiteness of the matrix B in (1.11). First, we introduce some lemmas that will be used later.

Proposition 2.1 ([19, p. 28]). *A matrix $P \in \mathbb{R}^{n\times n}$ is said to be positive definite in $\mathbb{R}^n$ if $(Px, x) > 0$, $\forall x \in \mathbb{R}^n$, $x \neq 0$. A real matrix P of order n is positive definite if and only if its symmetric part $H = (P + P^T)/2$ is positive definite.*

Definition 2.1 ([6, p. 13]). *Let $n \times n$ Toeplitz matrix T_n be of the following form:*

$$T_n = \begin{bmatrix} t_0 & t_{-1} & \cdots & t_{2-n} & t_{1-n} \\ t_1 & t_0 & t_{-1} & \cdots & t_{2-n} \\ \vdots & t_1 & t_0 & \ddots & \vdots \\ t_{n-2} & \cdots & \ddots & \ddots & t_{-1} \\ t_{n-1} & t_{n-2} & \cdots & t_1 & t_0 \end{bmatrix},$$

i.e. $t_{i,j} = t_{i-j}$ and T_n is constant along its diagonals. Assume that the diagonals $\{t_k\}_{k=-n+1}^{n-1}$ are the Fourier coefficients of a function g, i.e.

$$t_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} g(x)e^{-ikx}dx.$$

Then the function $g(x) = \sum_{k=1-n}^{n-1} t_k e^{ikx}$ is called the generating function of T_n.

Lemma 2.1 ([6, p. 13-15] (Grenander-Szegö Theorem)). *Let T_n be given by above matrix with a generating function g, where g is a 2π-periodic continuous real-valued functions* *defined on* $[-\pi, \pi]$*. Let* $\lambda_{\min}(T_n)$ *and* $\lambda_{\max}(T_n)$ *denote the smallest and largest eigenvalues of* T_n*, respectively. Then we have*

$$g_{\min} \le \lambda_{\min}(T_n) \le \lambda_{\max}(T_n) \le g_{\max},$$

where $g_{\min}$ *and* $g_{\max}$ *is the minimum and maximum values of* $g(x)$*, respectively. Moreover, if* $g_{\min} < g_{\max}$*, then all eigenvalues of* T_n *satisfies*

$$g_{\min} < \lambda(T_n) < g_{\max}$$

for all $n > 0$*. In particular, if* $g_{\min} > 0$*, then* T_n *is positive definite.*

Lemma 2.2 ([19, p. 29] (Sylvester Criterion)). *Let* $P \in \mathbb{R}^{n\times n}$ *be symmetric. Then,* P *is positive definite if and only if the dominant principal minors of* P *are all positive.*

Lemma 2.3. *Let* $n \times n$ *matrices* $K_{n\times n}$ *and* $L_{n\times n}$ *with* $p_j \neq 0$ *be of the following form:*

$$K_{n\times n} = \begin{pmatrix} a_1 & b_2 & c_3 & & & \\ b_2 & a_2 & b_3 & \ddots & & \\ c_3 & b_3 & a_3 & \ddots & \ddots & \\ & \ddots & \ddots & \ddots & \ddots & c_n \\ & & \ddots & \ddots & \ddots & b_n \\ & & & c_n & b_n & a_n \end{pmatrix}, \quad L_{n\times n} = \begin{pmatrix} p_1 & q_2 & c_3 & & & \\ & p_2 & q_3 & \ddots & & \\ & & p_3 & \ddots & \ddots & \\ & & & \ddots & \ddots & c_n \\ & & & & p_{n-1} & q_n \\ & & & & & p_n \end{pmatrix}.$$

Then the dominant principal minors of K *are*

$$\det K_{j\times j} = \det L_{j\times j},$$

where

$$\begin{aligned} &p_1 = a_1, \quad q_2 = b_2, \quad p_2 = a_2 - \frac{1}{p_1} q_2^2, \\ &q_j = b_j - \frac{q_{j-1}}{p_{j-2}} c_j, \qquad p_j = a_j - \frac{1}{p_{j-2}} c_j^2 - \frac{1}{p_{j-1}} q_j^2, \quad j \ge 3. \end{aligned}$$

Proof. Using the elementary row operations, the desired result is obtained. □

2.1. Ratio estimate by Grenander-Szegö theorem

Let the diagonal matrix be

$$\Lambda = \mathrm{diag}(\tau_1, \tau_2, \cdots, \tau_n). \tag{2.1}$$

From (1.11), we have

$$A := \Lambda^{\frac{1}{2}} B \Lambda^{\frac{1}{2}} = \begin{pmatrix} a_0^{(1)} & & & & \\ a_1^{(2)} & a_0^{(2)} & & & \\ a_2^{(3)} & a_1^{(3)} & a_0^{(3)} & & \\ & \ddots & \ddots & \ddots & \\ & & a_2^{(n)} & a_1^{(n)} & a_0^{(n)} \end{pmatrix}. \tag{2.2}$$

Here the coefficients are computed by

$$
\begin{aligned}
a_0^{(1)} &= 1, \quad a_0^{(2)} = \frac{1+2r_2}{1+r_2}, \quad a_1^{(2)} = \frac{-r_2^{3/2}}{1+r_2}, \\
a_0^{(n)} &= \frac{(1+r_{n-1})\big[1+2r_n+r_{n-1}\big(1+4r_n+3r_n^2\big)\big]}{(1+r_n)(1+r_{n-1})(1+r_{n-1}+r_nr_{n-1})}, \\
a_1^{(n)} &= -\frac{r_n^{3/2}[(1+2r_{n-1}+r_nr_{n-1})^2-r_{n-1}(1+r_{n-1})]}{(1+r_n)(1+r_{n-1})(1+r_{n-1}+r_nr_{n-1})}, \\
a_2^{(n)} &= \frac{r_n^{3/2}r_{n-1}^{5/2}(1+r_n)^2}{(1+r_n)(1+r_{n-1})(1+r_{n-1}+r_nr_{n-1})}, \quad n \geq 3.
\end{aligned} \tag{2.3}
$$

We next estimate the upper adjacent time-step ratio in a sense of $r_{k-1} \equiv r_k$.

Lemma 2.4. *Let (constant) adjacent time-step ratio satisfy $r_k \leq r_{\max} = 1.716$, $k \geq 2$. Then the matrix A defined in (2.2) or B in (1.11) is positive semi-definite.*

Proof. Let $y = r_k \leq r_{\max} = 1.716$. We prove the desired result in the following two cases:

Case I: $r_k \leq 1$. Since

$$
\begin{aligned}
&2a_0^{(1)} - \big|a_1^{(2)}\big| - \big|a_2^{(3)}\big| \geq 2 - 1 - \frac{1}{3} = \frac{2}{3}, \\
&2a_0^{(2)} - \big|a_1^{(2)}\big| - \big|a_1^{(3)}\big| - \big|a_2^{(4)}\big| = \frac{1}{(1+y)(1+y+y^2)} g(y),
\end{aligned}
$$

where

$$
\begin{aligned}
g(y) &= 2(1+2y)(1+y+y^2) - y^{\frac{3}{2}}(1+y+y^2) - y^{\frac{3}{2}}[(1+y)^3 - y] - y^4 - y^5 \\
&\geq 2(1+2y)(1+y+y^2) - y(1+y+y^2) - y[(1+y)^3 - y] - y^4 - y^5 \\
&= 2 + 4y + 3y^2 - 2y^4 - y^5 \geq 2.
\end{aligned}
$$

Moreover, we have

$$
2a_0^{(n)} - 2\big|a_1^{(n)}\big| - 2\big|a_2^{(n)}\big| = \frac{2}{(1+y)(1+y+y^2)} g_1(y), \quad n \geq 3,
$$

where

$$
\begin{aligned}
g_1(y) &= (1+y)^3 + y^2 + 2y^3 - y^{\frac{3}{2}}(1+y)^3 + y^{\frac{5}{2}} - y^4 - y^5 \\
&\geq (1+y)^3(1-y) + y^2 \geq 1.
\end{aligned}
$$

From the above inequalities, we know that the symmetric matrix $A + A^T$ in (2.2) is a diagonally dominant matrix. Using the Gerschgorin circle theorem, the eigenvalues of $A + A^T$ are greater than zero, it implies that the matrix A is positive definite by Proposition 2.1.

Case II: $1 < r_k \leq r_{\max} = 1.716$. For any real sequence $\{w_k\}_{k=1}^n$, it holds that

$$
\begin{aligned}
2\omega_k \sum_{j=1}^{k} a_{k-j}^{(k)} \omega_j &= 2a_0^{(k)}\omega_k^2 + 2a_1^{(k)}\omega_k\omega_{k-1} + 2a_2^{(k)}\omega_k\omega_{k-2} \\
&= a_2^{(k)}\omega_k^2 + a_2^{(k)}\left(\frac{a_1^{(k)}}{2a_2^{(k)}}\omega_k + \omega_{k-1}\right)^2 - a_2^{(k)}\omega_{k-1}^2 - a_2^{(k)}\left(\frac{a_1^{(k)}}{2a_2^{(k)}}\omega_{k-1} + \omega_{k-2}\right)^2 \\
&\quad + 2\left(a_0^{(k)} - a_2^{(k)} - \frac{\big(a_1^{(k)}\big)^2}{8a_2^{(k)}}\right)\omega_k^2 + a_2^{(k)}\left(\omega_k + \frac{a_1^{(k)}}{2a_2^{(k)}}\omega_{k-1} + \omega_{k-2}\right)^2,
\end{aligned}
$$

where

$$a_0^{(k)} = a_0^{(3)}, \quad a_1^{(k)} = a_1^{(3)}, \quad a_2^{(k)} = a_2^{(3)}, \quad k \geq 3.$$

We can check that

$$a_0^{(k)} - a_2^{(k)} - \frac{\left(a_1^{(k)}\right)^2}{8a_2^{(k)}} = \frac{y^3}{8a_2^{(k)}(1+y)^2(1+y+y^2)^2} l(y) > 0, \quad 1 \leq y \leq 1.731 < \sqrt{3}, \tag{2.4}$$

since

$$\begin{aligned} l(y) &= -8y^7 - 17y^6 + 10y^5 + 43y^4 + 42y^3 + 22y^2 + 4y - 1 \\ &\geq y\left(10y^4 - 8r_{\max}^3 y^3 - 17r_{\max}^2 y^3 + 43y^3 + 42y^2 + 22y + 3\right) > 0. \end{aligned}$$

Using (2.3) and the above equations, we obtain

$$\begin{aligned} 2\sum_{k=1}^{n} \omega_k \sum_{j=1}^{k} a_{k-j}^{(k)} \omega_j &\geq \left(2a_0^{(1)} - a_2^{(3)}\right) w_1^2 + \left(2a_1^{(2)} - a_1^{(3)}\right) w_1 w_2 + \left(2a_0^{(2)} - a_2^{(3)} - \frac{\left(a_1^{(3)}\right)^2}{4a_2^{(3)}}\right) w_2^2 \\ &= (w_1, w_2) \begin{pmatrix} 2a_0^{(1)} - a_2^{(3)} & a_1^{(2)} - \frac{a_1^{(3)}}{2} \\ a_1^{(2)} - \frac{a_1^{(3)}}{2} & 2a_0^{(2)} - a_2^{(3)} - \frac{\left(a_1^{(3)}\right)^2}{4a_2^{(3)}} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \geq 0, \end{aligned}$$

since the dominant principal minors of the above 2×2 matrix are greater than zero if $1 < r_k \leq r_{\max} = 1.716$. The proof is complete. □

Remark 2.1. The generating function of BDF3 kernels $b_{n-k}^{(n)}$ in (1.4) is

$$\begin{aligned} g(x) &= a_0^{(n)} + a_1^{(n)} \cos\varphi + a_2^{(n)} \cos(2\varphi) \\ &= 2a_2^{(n)} x^2 + a_1^{(n)} x + \left(a_0^{(n)} - a_2^{(n)}\right), \quad n \geq 3, \end{aligned} \tag{2.5}$$

where $\cos\varphi = x, x \in [-1, 1], \varphi \in [-\pi, \pi]$. From $2a_2^{(n)} > 0$ and (2.4), it implies that $g(x) > 0$ if $1 < r_k \leq 1.731$. Then BDF3 kernels $b_{n-k}^{(n)}$ in (1.4) are positive definite by Lemma 2.1. In fact, combining with the proof process of Case I in Lemma 2.4, the BDF3 kernels $b_{n-k}^{(n)}$ in (1.4) are positive definite if $r_k \leq 1.731 < \sqrt{3}$.

2.2. Ratio estimate by Sylvester criterion

From Section 2.1, we know that the matrix A in (2.2) is positive semi-definite with $r_s \leq 1.716$. Moreover, the BDF3 kernels $b_{n-k}^{(n)}$ in (1.4) are positive definite if $r_k \leq 1.731 < \sqrt{3}$ in (2.5). In fact, we can check that the generating function $g(x) < 0$ in (2.5) if $x = 0.434$, $r_k = 1.732$. However, the positive definiteness with $r_k = 1.732$ in (1.4) by Grenander-Szegö theorem is still in doubt. Therefore, we need to look for the upper bound estimate of other forms.

Let A be given in (2.2). From Lemma 2.3, the dominant principal minors of $A + A^T$ are

$$\det(A + A^T)_{k\times k} = \det L_{k\times k}.$$

Here the coefficients of $L_{k\times k}$ are

$$p_1 = 2a_0^{(1)}, \quad q_2 = a_1^{(2)}, \quad p_2 = 2a_0^{(2)} - \frac{1}{p_1} q_2^2, \tag{2.6a}$$

$$q_j = a_1^{(j)} - \frac{q_{j-1}}{p_{j-2}} a_2^{(j)}, \quad p_j = 2a_0^{(j)} - \frac{1}{p_{j-2}} \big(a_2^{(j)}\big)^2 - \frac{1}{p_{j-1}} q_j^2, \quad j \geq 3. \tag{2.6b}$$

As a counterexample, we take $r_s := r_n = r_{n-1} < \sqrt{3}$ in (2.6). According to Sylvester criterion in Lemma 2.2 and (2.6), we know that there exists a dominant principal minor of $A + A^T$ is negative, since there exists $p_j < 0$, see Fig. 2.1. Hence, the matrix A in (2.2) or B in (1.11) is not positive definite if $r_s = 1.732 < \sqrt{3}$.

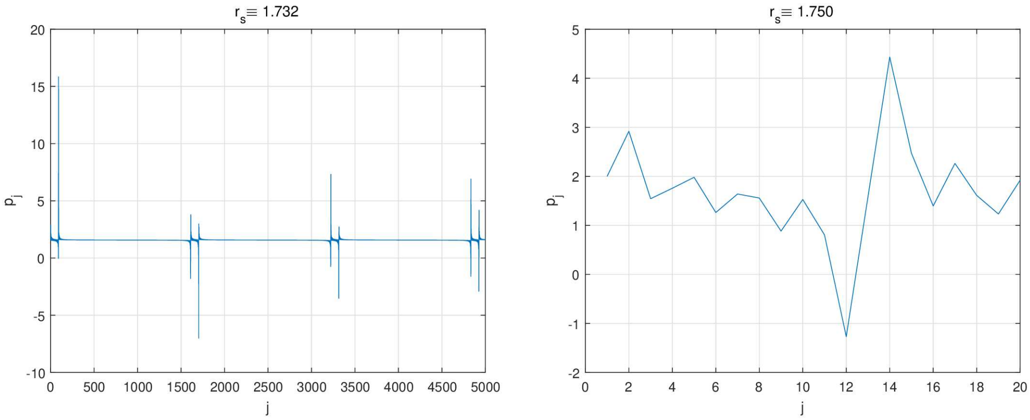

Fig. 2.1. The graphs of p_j in (2.6), left and right, respectively, for $r_s \equiv 1.732$ and $r_s \equiv 1.750$.

3. Estimate of Variable Adjacent Time-Step Ratio

From Section 2, the upper bound of fixed adjacent time-step ratio is less than $\sqrt{3}$ in a sense of the positive semi-definiteness of the matrix B in (1.11). However, it is not easy to obtain an sharp estimate for the general (variable) adjacent time-step ratio. In this section, we prove the variable adjacent time-step ratio $r_k \leq 1.405$, which plays an important role in our numerical analysis for the variable steps BDF3 scheme (1.7).

Let B and Λ be given in (1.11) and (2.1), respectively. Let

$$\widetilde{B} = B - \gamma \Lambda^{-1}, \quad \gamma = \frac{1}{200}. \tag{3.1}$$

From Lemma 2.3, the dominant principal minors of $\widetilde{B} + \widetilde{B}^T$ are

$$\det \big(\widetilde{B} + \widetilde{B}^T\big)_{j \times j} = \det L_{j \times j}.$$

Here the coefficients of L are computed by

$$\begin{aligned} &p_1 = \widehat{b}_0^{(1)}, \quad q_2 = b_1^{(2)}, \quad p_2 = \widehat{b}_0^{(2)} - \frac{1}{p_1} q_2^2, \\ &q_j = b_1^{(j)} - \frac{q_{j-1}}{p_{j-2}} b_2^{(j)}, \quad p_j = \widehat{b}_0^{(j)} - \frac{1}{p_{j-2}} \big(b_2^{(j)}\big)^2 - \frac{1}{p_{j-1}} q_j^2, \quad j \geq 3, \end{aligned} \tag{3.2}$$

where

$$\widehat{b}_0^{(1)} = \frac{1.99}{\tau_1}, \quad \widehat{b}_0^{(2)} = \frac{1.99 + 3.99 r_2}{\tau_2(1 + r_2)}, \quad b_1^{(2)} = \frac{-r_2^2}{\tau_2(1 + r_2)}, \tag{3.3a}$$

$$\widehat{b}_0^{(n)} = \frac{(1+r_{n-1})\big[1.99+3.99r_n+r_{n-1}\big(1.99+7.98r_n+5.99r_n^2\big)\big]}{\tau_n(1+r_n)(1+r_{n-1})(1+r_{n-1}+r_nr_{n-1})}, \tag{3.3b}$$

$$b_1^{(n)} = -\frac{r_n^2\big[(1+2r_{n-1}+r_nr_{n-1})^2-r_{n-1}(1+r_{n-1})\big]}{\tau_n(1+r_n)(1+r_{n-1})(1+r_{n-1}+r_nr_{n-1})}, \tag{3.3c}$$

$$b_2^{(n)} = \frac{r_n^2r_{n-1}^3(1+r_n)^2}{\tau_n(1+r_n)(1+r_{n-1})(1+r_{n-1}+r_nr_{n-1})}, \quad n\ge 3. \tag{3.3d}$$

The main aim of this part is to estimate the following inequality:

$$\frac{\lambda_{\min}}{\tau_j} \le p_j \le \frac{\lambda_{\max}}{\tau_j}, \quad j\ge 1, \quad \lambda_{\min}=1.99, \quad \lambda_{\max}=3.99,$$

it implies that the matrix A in (2.2) or B in (1.11) is positive definite by Sylvester criterion.

3.1. A few technical lemmas

First, we give some lemmas that will be used later.

Lemma 3.1. *Let $\Psi(x,y)$ with $(x,y)\in[0,r_s]\times[0,r_s], r_s=1.405$ be defined by*

$$\Psi(x,y) = \frac{(1+2y+xy)^2-y(1+y)}{(1+y)(1+y+xy)} - \frac{\kappa y^4(1+x)^2}{(1+y)^2(1+y+xy)}.$$

Here the coefficients are defined by

$$\kappa\in[\kappa_{\min},\kappa_{\max}], \quad \kappa_{\min}=0.25, \quad \kappa_{\max}=1.4.$$

Then we have

$$1\le\Psi(x,y)\le 2.7.$$

Proof. We can check that

$$\begin{aligned}\Psi(x,y) &= 1+\frac{(y^2+y^3-\kappa y^4)(1+x)^2+(1+x)y(1+y)^2}{(1+y)^2(1+y+xy)}\\ &= 1+\frac{(y^2+3y^3/2-\kappa y^4)(1+x)^2+(1+x)y(1+y)^2-y^3(1+x)^2/2}{(1+y)^2(1+y+xy)}\\ &= 1+\frac{(y^2+3y^3/2-\kappa y^4)(1+x)^2+(1-x^2)y^3/2+(2+2x)y^2+(1+x)y}{(1+y)^2(1+y+xy)} \ge 1.\end{aligned}$$

Here we use

$$y^2+\frac{3}{2}y^3-\kappa y^4 = y^2\left(1+\frac{3}{2}y-\kappa y^2\right) \ge y^2\left(1-\frac{3}{2}y(y-1)\right)\ge 0,$$

and

$$\begin{aligned}&\frac{1}{2}(1-x^2)y^3+(2+2x)y^2+(1+x)y\\ &=(1+x)y\left(\frac{1}{2}(1-x)y^2+2y+1\right)\\ &\ge(1+x)y(-0.3y^2+2y+1)\ge 0.\end{aligned}$$

Similarly, we have

$$\Psi(x,y) = 2.7 + \frac{(y^3 - y^2 - \kappa y^4)(1+x)^2 + \Psi_1(x,y)}{(1+y)^2(1+y+xy)},$$

where the quadratic function $\Psi_1(x,y)$ is

$$\begin{aligned}\Psi_1(x,y) &= -1.7(1+y)^3 + y(1+y)^2 - 0.7xy(1+y)^2 + 2y^2(1+x)^2 \\ &\leq -1.7(1+y)^2(y/1.405 + y) + y(1+y)^2 - 0.7xy(1+y)^2 + 4.81y^2(1+x) \\ &\leq -2.909y(1+y)^2 + y(1+y)^2 - 0.7xy(1+y)^2 + 4.81y^2(1+x) = y\Psi_2(x,y),\end{aligned}$$

where

$$\Psi_2(x,y) = -(1.909 + 0.7x)y^2 + (0.992 + 3.41x)y - 1.909 - 0.7x.$$

Since the discriminant of root formulas of $\Psi_2(x,y)$ is

$$\Delta = (0.992 + 3.41x)^2 - 4(1.909 + 0.7x)(1.909 + 0.7x) < 0,$$

which implies $\Psi_1(x,y) \leq 0$. Moreover, we have

$$y^3 - y^2 - \kappa y^4 = y^2(-\kappa y^2 + y - 1) \leq y^2(-0.25y^2 + y - 1) \leq 0.$$

The proof is complete. □

Lemma 3.2. *Let $\psi(x,y)$ with $(x,y) \in [0,r_s] \times [0,r_s], r_s = 1.405$ be defined by*

$$\psi(x,y) = -\frac{x^2[(1+2y+xy)^2 - y(1+y)]}{(1+x)(1+y)(1+y+xy)} + \frac{\kappa_{\max} x^2 y^4 (1+x)}{(1+y)^2(1+y+xy)}, \quad \kappa_{\max} = 1.4.$$

Then we have $\psi(x,y) \leq 0$.

Proof. We can check

$$\psi(x,y) = \frac{x^2}{(1+x)(1+y)^2(1+y+xy)}\psi_1(x,y),$$

where

$$\psi_1(x,y) = -(1+y)^3 - 2y(1+x)(1+y)^2 - y^2(1+x)^2(1+y) + y(1+y)^2 + 1.4y^4(1+x)^2.$$

Using the above equation and $1.4y - 2 < 0$, it yields

$$\begin{aligned}\psi_1(x,y) &\leq -2y(1+x)(1+y)^2 - y^2(1+x)^2(1+y) + y(1+y)^2 + 1.4y^3(1+y)(1+x)^2 \\ &= y(1+y)\big[-2(1+x)(1+y) + y(1+x)^2 + (1+y) + (1.4y-2)y(1+x)^2\big] \\ &\leq y(1+y)\psi_2(x,y),\end{aligned}$$

where

$$\psi_2(x,y) = -2(1+x)(1+y) + y(1+x)^2 + (1+y).$$

Since the first derivative of $\psi_2(x,y)$ with respect to y is greater than zero. Then we have $\psi_2(x,y) \leq \psi_2(x,r_s) < 0$. The proof is complete. □

Lemma 3.3. *Let* $\Phi(x,y)$ *with* $(x,y)\in[0,r_s]\times[0,r_s], r_s=1.405$ *be defined by*

$$\begin{aligned}\Phi(x,y)=&[1.99+3.99x+y(1.99+7.98x+5.99x^2)](1+x)(1+y)^4(1+y+xy)\\&-\lambda_{\min}(1+x)^2(1+y)^4(1+y+xy)^2-\frac{1}{\lambda_{\min}}x^3y^5(1+x)^4(1+y)^2\\&-\frac{1}{\lambda_{\min}}x^3\left[(1+2y+2xy)(1+y)^2+y^2(1+x)^2\left(1+y-\kappa_{\min}y^2\right)\right]^2,\end{aligned}$$

where $\lambda_{\min}=1.99$, $\kappa_{\min}=0.25$. *Then we have* $\Phi(x,y)\geq 0$.

Proof. According to

$$\begin{aligned}&1\leq 1+y-\kappa_{\min}y^2\leq 1+r_s-\kappa_{\min}r_s^2<1.912,\\&1.99+3.99x+y\left(1.99+7.98x+5.99x^2\right)-\lambda_{\min}(1+x)(1+y+xy)\\=&2x(1+2y+2xy),\end{aligned}$$

it leads to

$$\begin{aligned}\lambda_{\min}\Phi(x,y)\geq&3.98x\left(1+2y+2xy\right)(1+x)(1+y)^4(1+y+xy)-x^3y^5(1+x)^4(1+y)^2\\&-x^3\left[(1+2y+2xy)(1+y)^2+1.912y^2(1+x)^2\right]^2\\=&x(1+y)^4\Phi_1(x,y)+xy(1+x)(1+y)^2\Phi_2(x,y)+xy^2(1+x)^2\Phi_3(x,y).\end{aligned}$$

Here

$$\begin{aligned}\Phi_1(x,y)=&-1.13x^2y(1+x)-x^2+3.98x+3.98,\\\Phi_2(x,y)=&11.94(1+x)(1+y)^2-2.87x^2(1+y)^2\\&-2.793x^2y(1+x)(1+y)^2-3.824x^2y(1+x),\\\Phi_3(x,y)=&7.96(1+x)(1+y)^4-1.207x^2(1+y)^4-x^2y^3(1+x)^2(1+y)^2\\&-7.648x^2y(1+x)(1+y)^2-3.655744x^2y^2(1+x)^2.\end{aligned}$$

We can check

$$\begin{aligned}\Phi_1(x,y)\geq&-1.13x^2r_s(1+r_s)-x^2+3.98x+3.98>0,\\\Phi_2(x,y)\geq&11.94(1+x)(1+y)^2-2.87x^2(1+y)^2-6.718x^2y(1+y)^2-9.197x^2y\\=&x(1+y)^2(11.94-6.048xy)+h(x,y)\geq h(x,y),\end{aligned}$$

where

$$h(x,y)=11.94(1+y)^2-2.87x^2(1+y)^2-0.67x^2y(1+y)^2-9.197x^2y.$$

Since the first derivative of $h(x,y)$ with respect to x is less than zero. It implies that $h(x,y)\geq h(r_s,y)$. Moreover, the first derivative of $h(r_s,y)$ with respect to y is also less than zero. Then

$$\Phi_2(x,y)\geq h(x,y)\geq h(r_s,y)\geq h(r_s,r_s)>0.$$

On the other hand, there exists

$$\Phi_3(x,y)\geq xg(x,y),$$

where

$$g(x,y)=7.96\left(\frac{1}{r_s}+1\right)(1+y)^4-1.207x(1+y)^4-xy^3(1+r_s)^2(1+y)^2$$

$$- 7.648xy(1 + r_s)(1 + y)^2 - 3.655744xy^2(1 + r_s)^2.$$

Since the first derivative of $g(x, y)$ with respect to x is less than zero. It implies $g(x, y) \geq g(r_s, y)$. Furthermore, we have $g(r_s, y) \geq g(r_s, r_s) > 0$. Hence, there exists

$$\Phi_3(x, y) \geq xg(x, y) \geq xg(r_s, y) \geq xg(r_s, r_s) \geq 0.$$

The proof is complete. □

Lemma 3.4. *Let $\phi(x, y)$ with $(x, y) \in [0, r_s] \times [0, r_s], r_s = 1.405$ be defined by*

$$\begin{aligned}\phi(x, y) = {} & [1.99 + 3.99x + y(1.99 + 7.98x + 5.99x^2)](1 + x)(1 + y)^4(1 + y + xy) \\ & - \lambda_{\max}(1 + x)^2(1 + y)^4(1 + y + xy)^2 - \frac{1}{\lambda_{\max}} x^3y^5(1 + x)^4(1 + y)^2 \\ & - \frac{1}{\lambda_{\max}} x^3 \left[(1 + 2y + 2xy)(1 + y)^2 + y^2(1 + x)^2\big(1 + y - \kappa_{\max}y^2\big)\right]^2,\end{aligned}$$

where $\lambda_{\max} = 3.99$, $\kappa_{\max} = 1.4$. Then we have $\phi(x, y) \leq 0$.

Proof. Using

$$\begin{aligned}& \big[(2y + 2xy)(1 + y)^2 + y^2(1 + x)^2\big(1 + y - \kappa_{\max}y^2\big)\big] - 2y^2(1 + x)(1 + y) \\ \geq {} & y(1 + x)\big[2(1 + y)^2 + y\big(1 + y - \kappa_{\max}y^2\big) - 2y(1 + y)\big] \geq 0,\end{aligned}$$

and

$$1.99 + 3.99x + y(1.99 + 7.98x + 5.99x^2) - \lambda_{\max}(1 + x)(1 + y + xy) = -2 - 2y + 2x^2y,$$

it yields

$$\begin{aligned}\lambda_{\max}\phi(x, y) & \leq \lambda_{\max}(-2 - 2y + 2x^2y)(1 + x)(1 + y)^4(1 + y + xy) - 4x^3y^4(1 + x)^2(1 + y)^2 \\ & = (1 + x)^2(1 + y)^2y\phi_1(x, y) + (1 + x)(1 + y)^4\phi_2(x, y).\end{aligned}$$

Here the functions $\phi_1(x, y)$ and $\phi_2(x, y)$ are respectively defined by

$$\begin{aligned}\phi_1(x, y) & = 7.98x^2y(1 + y)^2 - 7(1 + y)^3 - 4x^3y^3, \\ \phi_2(x, y) & = 7.98x^2y - 7.98(1 + y) - 0.98y(1 + y)(1 + x) \leq \phi_3(x, y),\end{aligned}$$

where

$$\phi_3(x, y) = 7.98x^2y - 7.98(1 + y) - 0.98y(1 + y).$$

Since the first derivative of $\phi_1(x, y)$ and $\phi_3(x, y)$ with respect to x is greater than zero. Hence,

$$\begin{aligned}\phi_1(x, y) \leq \phi_1(r_s, y) \leq \phi_1(r_s, r_s) \leq 0, \\ \phi_3(x, y) \leq \phi_3(r_s, y) \leq \phi_3(r_s, r_s) \leq 0.\end{aligned}$$

The proof is complete. □

3.2. Estimate for variable time-step ratio by Sylvester criterion

We next prove the matrix A in (2.2) or B in (1.11) is positive definite by Sylvester criterion.

Lemma 3.5. *Let p_j and q_j be defined by (3.2). Then for any adjacent time-step ratios $0<r_k \le r_s = 1.405, k \ge 2$, there exists*

$$b_1^{(j)} + \mu_j \le q_j \le b_1^{(j)} + \nu_j \le 0, \quad j \ge 3, \tag{3.4}$$

where

$$\begin{aligned} \mu_j &= \frac{\kappa_{\min} r_j^2 r_{j-1}^4 (1+r_j)}{\tau_j (1+r_{j-1})^2 (1+r_{j-1}+r_j r_{j-1})}, \\ \nu_j &= \frac{\kappa_{\max} r_j^2 r_{j-1}^4 (1+r_j)}{\tau_j (1+r_{j-1})^2 (1+r_{j-1}+r_j r_{j-1})}, \end{aligned} \tag{3.5}$$

and

$$\frac{\lambda_{\min}}{\tau_j} \le p_j \le \frac{\lambda_{\max}}{\tau_j}, \quad j \ge 1. \tag{3.6}$$

Here the coefficients are defined by

$$\kappa_{\min} = 0.25, \quad \kappa_{\max} = 1.4, \quad \lambda_{\min} = 1.99, \quad \lambda_{\max} = 3.99.$$

Proof. From (3.2) and (3.3), we obtain

$$p_1 = \frac{1.99}{\tau_1}, \quad q_2 = \frac{-r_2^2}{\tau_2(1+r_2)},$$

and

$$\begin{aligned} \frac{\lambda_{\max}}{\tau_2} &\ge \frac{\lambda_{\max}}{\tau_2} - \frac{2+2r_2+(1/1.99)r_2^3}{\tau_2(1+r_2)^2} = p_2 \\ &= \frac{\lambda_{\min}}{\tau_2} + \frac{2r_2+2r_2^2-(1/1.99)r_2^3}{\tau_2(1+r_2)^2} \ge \frac{\lambda_{\min}}{\tau_2}. \end{aligned}$$

Next we prove (3.4) and (3.6) by mathematical induction.

For $j=3$, using Lemma 3.2, we have

$$b_1^{(3)} + \mu_3 \le b_1^{(3)} + \frac{(1/1.99) r_2^4 r_3^2 (1+r_3)}{\tau_3 (1+r_2)^2 (1+r_2+r_2 r_3)} = q_3 \le b_1^{(3)} + \nu_3 = \psi(r_3, r_2) \le 0. \tag{3.7}$$

According to (3.2), (3.3) and (3.7), it yields

$$\begin{aligned} p_3 &\ge \widehat{b}_0^{(3)} - \frac{\tau_1}{\lambda_{\min}} \big(b_2^{(3)}\big)^2 - \frac{\tau_2}{\lambda_{\min}} \big(b_1^{(3)} + \mu_3\big)^2 \\ &= \frac{\lambda_{\min}}{\tau_3} + \frac{1}{\tau_3 (1+r_3)^2 (1+r_2)^4 (1+r_2+r_2 r_3)^2} \cdot \Phi(r_3, r_2) \ge \frac{\lambda_{\min}}{\tau_3} \end{aligned}$$

with $\Phi(r_3, r_2) \ge 0$ in Lemma 3.3.

On the other hand, using (3.2), (3.3) and (3.7), one has

$$\begin{aligned} p_3 &\le \widehat{b}_0^{(3)} - \frac{\tau_1}{\lambda_{\max}} \big(b_2^{(3)}\big)^2 - \frac{\tau_2}{\lambda_{\max}} \big(b_1^{(3)} + \nu_3\big)^2 \\ &= \frac{\lambda_{\max}}{\tau_3} + \frac{1}{\tau_3 (1+r_3)^2 (1+r_2)^4 (1+r_2+r_2 r_3)^2} \cdot \phi(r_3, r_2) \le \frac{\lambda_{\max}}{\tau_3} \end{aligned}$$

with $\phi(r_3, r_2) \le 0$ in Lemma 3.4.

Supposing that (3.4) and (3.6) hold for $j = 4, \dots, n-1$, namely,

$$b_1^{(j)} + \mu_j \le q_j \le b_1^{(j)} + \nu_j \le 0, \quad \frac{\lambda_{\min}}{\tau_j} \le p_j \le \frac{\lambda_{\max}}{\tau_j}, \quad 4 \le j \le n-1. \tag{3.8}$$

According to (3.2), (3.3), (3.8) and Lemma 3.2, there exists

$$\begin{aligned}
q_n &= b_1^{(n)} - \frac{q_{n-1}}{p_{n-2}} b_2^{(n)} \le b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\min}} (-q_{n-1})\, b_2^{(n)} \\
&\le b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\min}} \big(- b_1^{(n-1)} - \mu_{n-1} \big) b_2^{(n)} \\
&= b_1^{(n)} + \frac{\Psi(r_{n-1}, r_{n-2})}{\lambda_{\min}} \frac{r_n^2 r_{n-1}^4 (1 + r_n)}{\tau_n (1 + r_{n-1})^2 (1 + r_{n-1} + r_n r_{n-1})} \\
&\le b_1^{(n)} + \nu_n = \psi(r_n, r_{n-1}) \le 0,
\end{aligned}$$

where $\Psi(r_{n-1}, r_{n-2})$ and ν_n are, respectively, defined by Lemma 3.1 and (3.5). On the other hand, using (3.2), (3.3) and (3.8), we have

$$\begin{aligned}
q_n &= b_1^{(n)} - \frac{q_{n-1}}{p_{n-2}} b_2^{(n)} \ge b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\max}} (-q_{n-1}) b_2^{(n)} \\
&\ge b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\max}} \big(- b_1^{(n-1)} - \nu_{n-1} \big) b_2^{(n)} \\
&= b_1^{(n)} + \frac{\Psi(r_{n-1}, r_{n-2})}{\lambda_{\max}} \frac{r_n^2 r_{n-1}^4 (1 + r_n)}{\tau_n (1 + r_{n-1})^2 (1 + r_{n-1} + r_n r_{n-1})} \ge b_1^{(n)} + \mu_n,
\end{aligned}$$

where $\Psi(r_{n-1}, r_{n-2})$ and μ_n are, respectively, defined by Lemma 3.1 and (3.5).

From (3.2), (3.3) and (3.8), it yields

$$\begin{aligned}
p_n &= \widehat{b}_0^{(n)} - \frac{1}{p_{n-2}} \big(b_2^{(n)}\big)^2 - \frac{1}{p_{n-1}} q_n^2 \ge b_0^{(n)} - \frac{\tau_{n-2}}{\lambda_{\min}} \big(b_2^{(n)}\big)^2 - \frac{\tau_{n-1}}{\lambda_{\min}} \big(b_1^{(n)} + \mu_n\big)^2 \\
&= \frac{\lambda_{\min}}{\tau_n} + \frac{1}{\tau_n (1 + r_n)^2 (1 + r_{n-1})^4 (1 + r_{n-1} + r_{n-1} r_n)^2} \cdot \Phi(r_n, r_{n-1}) \ge \frac{\lambda_{\min}}{\tau_n}
\end{aligned}$$

with $\Phi(r_n, r_{n-1}) \ge 0$ in Lemma 3.3. Similarly, we have

$$\begin{aligned}
p_n &= \widehat{b}_0^{(n)} - \frac{1}{p_{n-2}} \big(b_2^{(n)}\big)^2 - \frac{1}{p_{n-1}} q_n^2 \le b_0^{(n)} - \frac{\tau_{n-2}}{\lambda_{\max}} \big(b_2^{(n)}\big)^2 - \frac{\tau_{n-1}}{\lambda_{\max}} \big(b_1^{(n)} + \nu_n\big)^2 \\
&= \frac{\lambda_{\max}}{\tau_n} + \frac{1}{\tau_n (1 + r_n)^2 (1 + r_{n-1})^4 (1 + r_{n-1} + r_{n-1} r_n)^2} \cdot \phi(r_n, r_{n-1}) \le \frac{\lambda_{\max}}{\tau_n}
\end{aligned}$$

with $\phi(r_n, r_{n-1}) \le 0$ in Lemma 3.4. The proof is complete. □

Remark 3.1. In fact, the upper ratio $r_s = 1.405$ is the root of the polynomial function $\Phi(x, x)$ arising from Lemma 3.3.

4. The Unique Solvability and Energy Stability

In this section, we show the unique solvability and discrete energy stability. Let $H^m(\Omega)$ and $\|\cdot\|_{H^m(\Omega)}$ denote the standard Sobolev spaces and their norms, respectively. In particular, let $(\cdot,\cdot)$ and $\|\cdot\|$ be the usual inner product and norm in the space $L^2(\Omega)$, respectively.

4.1. The unique solvability

First, we show the unique solvability of the BDF3 scheme (1.7) via a discrete energy functional for the Allen-Cahn equation (1.1).

Theorem 4.1. *If the time-step size*

$$\tau_n < \frac{1+2r_n+r_{n-1}(1+4r_n+3r_n^2)}{(1+r_n)(1+r_{n-1}+r_nr_{n-1})},$$

the variable-steps BDF3 scheme (1.7) *is uniquely solvable.*

Proof. For any fixed time-level indexes $n \geq 1$, we consider the following energy functional:

$$G[z] := \frac{b_0^{(n)}}{2}\|z-u^{n-1}\|^2 + \big(b_1^{(n)}\nabla_\tau u^{n-1} + b_2^{(n)}\nabla_\tau u^{n-2}, z-u^{n-1}\big) + \frac{\varepsilon^2}{2}\|\nabla z\|^2 + \frac{1}{4}\|z^2-1\|^2.$$

Under the time-step size condition

$$\tau_n < \frac{1+2r_n+r_{n-1}(1+4r_n+3r_n^2)}{(1+r_n)(1+r_{n-1}+r_nr_{n-1})}$$

or $b_0^{(n)} > 1$, the functional G is strictly convex. In fact, for any $\lambda \in \mathbb{R}$ and ψ, one has

$$\frac{d^2G}{d\lambda^2}[z+\lambda\psi]\Big|_{\lambda=0} = b_0^{(n)}\|\psi\|^2 + \varepsilon^2\|\nabla\psi\|^2 + 3\|z\psi\|^2 - \|\psi\|^2 \geq \big(b_0^{(n)}-1\big)\|\psi\|^2 > 0.$$

Thus, the functional G has a unique minimizer, denoted by u^n, if and only if it solves

$$0 = \frac{dG}{d\lambda}[z+\lambda\psi]\Big|_{\lambda=0} = \Big(b_0^{(n)}(z-u^{n-1}t) + b_1^{(n)}\nabla_\tau u^{n-1} + b_2^{(n)}\nabla_\tau u^{n-2} - \varepsilon^2\Delta z + f(z), \psi\Big).$$

This equation holds for any ψ if and only if the unique minimizer u^n solves

$$b_0^{(n)}(u^n-u^{n-1}) + b_1^{(n)}\nabla_\tau u^{n-1} + b_2^{(n)}\nabla_\tau u^{n-2} - \varepsilon^2\Delta u^n + f(u^n) = 0,$$

which is just the BDF3 scheme (1.7). The proof is complete. □

4.2. The discrete energy dissipation law

From (3.1) and Lemma 3.5, for any real sequence $\{w_k\}_{k=1}^n$, it holds that

$$\sum_{k=1}^n w_k \sum_{j=1}^k b_{k-j}^{(k)} w_j \geq \gamma \sum_{k=1}^n \frac{w_k^2}{\tau_k}, \quad n \geq 1. \tag{4.1}$$

Let $E(u^n)$ be the discrete version of free energy functional (1.2), given by

$$E(u^n) = \frac{\varepsilon^2}{2}\|\nabla u^n\|^2 + \frac{1}{4}\|(u^n)^2-1\|^2, \quad 0 \leq n \leq N. \tag{4.2}$$

Next theorem shows that the variable steps BDF3 scheme (1.7) preserves an energy dissipation law at the discrete levels, which implies the energy stability.

Theorem 4.2. *Let $r_n \le 1.405$. If the time-step sizes are properly small such that*

$$\tau_n \le \min\left\{ \frac{1+2r_n + r_{n-1}\left(1+4r_n+3r_n^2\right)}{(1+r_n)(1+r_{n-1}+r_n r_{n-1})}, 2\gamma \right\}, \quad n \ge 1. \tag{4.3}$$

Then the variable-steps BDF3 scheme (1.7) *preserves the following energy dissipation law:*

$$E(u^n) \le E(u^0), \quad n \ge 1. \tag{4.4}$$

Proof. The first condition of (4.3) ensures the unique solvability. We will establish the energy dissipation law under the second condition of (4.3). Making the inner product of (1.7) by $\nabla_\tau u^k$, we obtain

$$\left(D_3 u^k, \nabla_\tau u^k\right) - \varepsilon^2 \left(\Delta u^k, \nabla_\tau u^k\right) + \left(f(u^k), \nabla_\tau u^k\right) = 0. \tag{4.5}$$

With the help of the inequality $2a(a-b) \ge a^2 - b^2$, the second term in (4.5) reads

$$-\varepsilon^2 \left(\Delta u^k, \nabla_\tau u^k\right) = \varepsilon^2 \left(\nabla u^k, \nabla u^k - \nabla u^{k-1}\right) \ge \frac{\varepsilon^2}{2}\|\nabla u^k\|^2 - \frac{\varepsilon^2}{2}\|\nabla u^{k-1}\|^2.$$

It is easy to check the following identity:

$$4(a^3-a)(a-b) = (a^2-1)^2 - (b^2-1)^2 - 2(a-b)^2 + 2a^2(a-b)^2 + (a^2-b^2)^2.$$

Then the third term in (4.5) can be bounded by

$$\left(f(u^k), \nabla_\tau u^k\right) \ge \frac{1}{4}\left\| \left(u^k\right)^2 - 1\right\|^2 - \frac{1}{4}\left\|(u^{k-1})^2 - 1\right\|^2 - \frac{1}{2}\|u^k - u^{k-1}\|^2.$$

From (4.5) and the above inequalities, it yields

$$\left(D_3 u^k, \nabla_\tau u^k\right) + E(u^k) - E(u^{k-1}) - \frac{1}{2}\|u^k - u^{k-1}\|^2 \le 0, \quad k \ge 1.$$

Summing the above inequality from $k=1$ to n, we have

$$\sum_{k=1}^n \left(D_3 u^k, \nabla_\tau u^k\right) + E(u^n) - E(u^0) - \frac{1}{2}\sum_{k=1}^n \|u^k - u^{k-1}\|^2 \le 0.$$

According to (1.8) and (4.1), we obtain

$$\sum_{k=1}^n \left(D_3 u^k, \nabla_\tau u^k\right) = \sum_{k=1}^n \left(\sum_{j=1}^k b_{k-j}^{(k)} \nabla_\tau u^j, \nabla_\tau u^k \right) \ge \gamma \sum_{k=1}^n \frac{\|u^k - u^{k-1}\|^2}{\tau_k}, \quad n \ge 1.$$

Hence, it implies

$$\sum_{k=1}^n \left(\frac{\gamma}{\tau_k} - \frac{1}{2}\right) \|u^k - u^{k-1}\|^2 + E(u^n) - E(u^0) \le 0.$$

The second condition of (4.3) gives the desired result (4.4). □

Lemma 4.1. *Let $r_n \le 1.405$. If the step sizes τ_n fulfill* (4.3)*, the solution of the variable steps BDF3 scheme* (1.7) *is bounded in the sense that*

$$\|u^n\|_{H^1(\Omega)} \le c_1 := \sqrt{4\varepsilon^{-2}E(u^0) + (2+\varepsilon^2)|\Omega|}, \quad n \ge 1,$$

where c_1 is dependent on the domain Ω and the starting value u^0, but independent of the time t_n, the time-step sizes τ_n and the time-step ratios r_n.

Proof. From the discrete energy dissipation law (4.4) and the definition (4.2), it yields

$$\begin{aligned}4E(u^0) &\geq 4E(u^n) = 2\varepsilon^2\|\nabla u^n\|^2 + \|(u^n)^2 - 1\|^2\\ &= 2\varepsilon^2\|\nabla u^n\|^2 + \|(u^n)^2 - 1 - \varepsilon^2\|^2 + 2\varepsilon^2\|u^n\|^2 - \varepsilon^2(2+\varepsilon^2)|\Omega|\\ &\geq 2\varepsilon^2\|\nabla u^n\|^2 + 2\varepsilon^2\|u^n\|^2 - \varepsilon^2(2+\varepsilon^2)|\Omega|.\end{aligned}$$

Thus, we obtain

$$(\|u^n\| + \|\nabla u^n\|)^2 \leq 2\|u^n\|^2 + 2\|\nabla u^n\|^2 \leq 4\varepsilon^{-2}E(u^0) + (2+\varepsilon^2)|\Omega|.$$

The proof is complete. □

5. Stability and Convergence Analysis

In this section, we show the L^2 norm unconditional stability and convergence of the variable-step BDF3 scheme (1.7) for the Allen-Cahn equation.

Denote $\langle\cdot,\cdot\rangle$ the classical Euclidean scalar product

$$\langle\mu,\nu\rangle = \nu^T\mu = \sum_{k=1}^{n}\mu^k\nu^k, \quad |\mu| = \langle\mu,\mu\rangle^{\frac{1}{2}},$$

where $\mu = (\mu^1, \mu^2, \cdots, \mu^n)^T$ and $\nu = (\nu^1, \nu^2, \cdots, \nu^n)^T$. From [19, pp. 23-24], we know that the spectral norm of the matrix $A \in \mathbb{R}^{n\times n}$ satisfies

$$|A\mu| \leq |A||\mu|, \quad |A| = \sqrt{\rho(A^TA)}. \tag{5.1}$$

Here the spectral radius $\rho(A)$ is denoted by the maximum module of the eigenvalues of A.

Definition 5.1. *Let A and B be two real $n\times n$ matrices. Then, $A > B$ ($\geq B$) if $A - B$ is positive definite (positive semi-definite).*

Let I be the $n\times n$ identity matrix and $\Lambda = \text{diag}(\tau_1, \tau_2, \cdots, \tau_n)$ in (2.1). Then we have the following results.

Lemma 5.1. *Let $B > c\Lambda^{-1}$, $c > 0$. Then $\mathscr{A} := \Lambda^{1/2}B\Lambda^{1/2} > cI$.*

Proof. Taking $x = \Lambda^{1/2}y$ with $x \neq 0$, it yields

$$0 < x^T(B - c\Lambda^{-1})x = y^T\Lambda^{\frac{1}{2}}(B - c\Lambda^{-1})\Lambda^{\frac{1}{2}}y = \big\langle\big(\Lambda^{\frac{1}{2}}B\Lambda^{\frac{1}{2}} - cI\big)y, y\big\rangle.$$

The proof is complete. □

Lemma 5.2 (Spectral Norm Inequality). *Let $A > cI$, $c > 0$. Then the spectral norm $|A^{-1}| < c^{-1}$.*

Proof. Since

$$\big\langle(A - cI)x, x\big\rangle = x^T(A - cI)x > 0, \quad \big\langle(A^T - cI)x, x\big\rangle = x^T(A^T - cI)x > 0, \quad \forall x \neq 0.$$

Using the classical Euclidean scalar product, it yields

$$\begin{aligned}0 < |(A-cI)x|^2 &= x^T(A^T-cI)(A-cI)x\\ &= x^T(A^TA-cA^T-cA+c^2I)x\\ &= x^T(A^TA-c^2I-cA^T-cA+2c^2I)x, \quad \forall x\neq 0.\end{aligned}$$

According to the above inequalities, we have

$$\big\langle (A^TA-c^2I)x,x\big\rangle > c\big\langle (A^T+A-2cI)x,x\big\rangle > 0, \quad \forall x\neq 0, \tag{5.2}$$

which implies that the matrix A^TA is symmetric positive definite. Let $\{\mu_i\}_{i=1}^n$ be an orthonormal set of eigenvectors of A^TA, i.e. $A^TA\mu_i=\lambda_i\mu_i$ with $0<\lambda_1\leq\lambda_2\leq\cdots\leq\lambda_n$. Thus, we obtain

$$x^TA^TAx=\sum_{i=1}^n c_i^2\lambda_i, \quad x^Tx=\sum_{i=1}^n c_i^2, \quad \forall x=\sum_{i=1}^n c_i\mu_i.$$

From (5.2) and the above equations, there exists

$$\big\langle \big(A^TA-c^2I\big)x,x\big\rangle = x^T\big(A^TA-c^2I\big)x=\sum_{i=1}^n c_i^2(\lambda_i-c^2)>0, \quad \forall x\neq 0,$$

which leads to $\lambda_1>c^2$. From (5.1), one has

$$\rho\big((A^TA)^{-1}\big)=\lambda_1^{-1}<\frac{1}{c^2}, \quad |A^{-1}|<c^{-1}.$$

The proof is complete. □

Lemma 5.3. *If the BDF3 discrete convolution kernels $b_{n-k}^{(n)}$ in (1.8) are positive definite, the DOC kernels $d_{n-k}^{(n)}$ in (1.9) are also positive definite. For any real sequence $\{\mu^k\}_{k=1}^n$, it holds that*

$$\langle D\mu,\mu\rangle=\sum_{k=1}^n\mu^k\sum_{j=1}^k d_{k-j}^{(k)}\mu^j\geq 0, \quad n\geq 1.$$

Proof. Let $\mu=(\mu^1,\mu^2,\cdots,\mu^n)^T\in\mathbb{R}^n$. We can check

$$\sum_{k=1}^n\mu^k\sum_{j=1}^k d_{k-j}^{(k)}\mu^j=\mu^TD\mu=\langle D\mu,\mu\rangle, \quad n\geq 1$$

with the matrix D in (1.11).

According to Lemma 3.5, we know that the matrix B is positive definite. Let $\forall\mu\in\mathbb{R}^n$, $\mu\neq 0$, it yields $\nu=B\mu\neq 0$. Then we have

$$\nu^TD\nu=\nu^TB^{-1}\nu=\mu^TB^TB^{-1}B\mu=\mu^TB^T\mu=\langle\mu,B\mu\rangle>0.$$

The proof is complete. □

A discrete Grönwall's inequality is needed in the following analysis.

Lemma 5.4 ([18]). *Let $\lambda\geq 0$ and the sequences $\{\xi_k\}_{k=0}^N$ and $\{V_k\}_{k=1}^N$ be nonnegative. If*

$$V_n\leq\lambda\sum_{j=1}^{n-1}\tau_jV_j+\sum_{j=0}^n\xi_j, \quad 1\leq n\leq N,$$

then it holds that

$$V_n\leq\exp(\lambda t_{n-1})\sum_{j=0}^n\xi_j, \quad 1\leq n\leq N.$$

5.1. Stability analysis

First, we show the L^2 norm stability analysis of the variable steps BDF3 scheme (1.7) for the Allen-Cahn model (1.1).

Theorem 5.1. *Let BDF3 kernels $b_{n-k}^{(n)}$ be defined in* (1.8) *with $B > \gamma\Lambda^{-1}$ in* (3.1)*. Then the discrete solution u^n of BDF3 scheme* (1.7) *is unconditionally stable in the L^2 norm*

$$\|\epsilon^n\| \le 2\exp\big(4\gamma^{-1}\widetilde{c}t_{n-1}\big)\|\epsilon^0\|, \quad n \ge 1.$$

Proof. Let ϵ^n be the solution perturbation $\epsilon^n = \widetilde{u}^n - u^n$ for $0 \le n \le N$. The perturbed equation is obtained

$$D_3\epsilon^j - \varepsilon^2\Delta\epsilon^j = f(u^j) - f(\widetilde{u}^j) = \widetilde{f}_u^j\epsilon^j, \quad j \ge 1, \tag{5.3}$$

where

$$\widetilde{f}_u^j = 1 - (u^j)^2 - u^j\widetilde{u}^j - (\widetilde{u}^j)^2.$$

Note that the solution estimates in Lemma 4.1 and $H^1 \subseteq L^\infty$, we have

$$\begin{aligned}\|\widetilde{f}_u^j\|_{L^\infty} &\le 1 + \|u^j\|_{L^\infty}^2 + \|u^j\|_{L^\infty}\|\widetilde{u}^j\|_{L^\infty} + \|\widetilde{u}^j\|_{L^\infty}^2 \\ &\le 1 + c_\Omega^2\|u^j\|_{H^1}^2 + c_\Omega^2\|u^j\|_{H^1}\|\widetilde{u}^j\|_{H^1} + c_\Omega^2\|\widetilde{u}^j\|_{H^1}^2 \\ &\le 1 + c_\Omega^2 c_1^2 + c_\Omega^2 c_1\widetilde{c_1} + c_\Omega^2\widetilde{c_1}^2 := \widetilde{c}, \quad j \ge 1,\end{aligned} \tag{5.4}$$

where $\|\widetilde{u}^j\|_{H^1} \le \widetilde{c_1}$ is similar to Lemma 4.1. Multiplying both sides of (5.3) by the DOC kernels $d_{k-j}^{(k)}$, and summing j from 1 to k, we derive

$$\sum_{j=1}^k d_{k-j}^{(k)} D_3\epsilon^j - \varepsilon^2\sum_{j=1}^k d_{k-j}^{(k)}\Delta\epsilon^j = \sum_{j=1}^k d_{k-j}^{(k)}\widetilde{f}_u^j\epsilon^j, \quad k \ge 1.$$

According to (1.8) and (1.10), it yields

$$\sum_{j=1}^k d_{k-j}^{(k)} D_3\epsilon^j = \sum_{j=1}^k d_{k-j}^{(k)}\sum_{l=1}^j b_{j-l}^{(j)}\nabla_\tau\epsilon^l = \sum_{l=1}^k \nabla_\tau\epsilon^l\sum_{j=l}^k d_{k-j}^{(k)} b_{j-l}^{(j)} = \nabla_\tau\epsilon^k, \quad k \ge 1. \tag{5.5}$$

Hence, we have

$$\nabla_\tau\epsilon^k - \varepsilon^2\sum_{j=1}^k d_{k-j}^{(k)}\Delta\epsilon^j = \sum_{j=1}^k d_{k-j}^{(k)}\widetilde{f}_u^j\epsilon^j, \quad k \ge 1.$$

Making the inner product of the above equality with ϵ^k and summing the derived equality from $k = 1$ to n, one obtains

$$\sum_{k=1}^n \big(\nabla_\tau\epsilon^k, \epsilon^k\big) + \varepsilon^2\sum_{k=1}^n\sum_{j=1}^k d_{k-j}^{(k)}(\nabla\epsilon^j, \nabla\epsilon^k) = \sum_{k=1}^n\sum_{j=1}^k d_{k-j}^{(k)}\big(\widetilde{f}_u^j\epsilon^j, \epsilon^k\big), \quad n \ge 1.$$

For the first term on the left hand, we have

$$\sum_{k=1}^n \big(\nabla_\tau\epsilon^k, \epsilon^k\big) \ge \frac{1}{2}\sum_{k=1}^n \big(\|\epsilon^k\|^2 - \|\epsilon^{k-1}\|^2\big) = \frac{1}{2}\big(\|\epsilon^n\|^2 - \|\epsilon^0\|^2\big),$$

where the inequality $2a(a-b) \ge a^2 - b^2$ has been used.

For the second term on the left hand, using Lemma 5.3, we obtain

$$\varepsilon^2 \sum_{k=1}^{n} \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\nabla \epsilon^j, \nabla \epsilon^k \right) \geq 0.$$

From the above estimates, (1.11), Lemma 5.1, discrete Cauchy-Schwarz inequality and (3.1), it yields

$$\begin{aligned}
\|\epsilon^n\|^2 - \|\epsilon^0\|^2 &\leq 2 \sum_{k=1}^{n} \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\widetilde{f}_u^j \epsilon^j, \epsilon^k \right) \\
&= 2 \int_\Omega \mathcal{E}^T D F_\epsilon dx = 2 \int_\Omega \langle D F_\epsilon, \mathcal{E} \rangle dx \\
&= 2 \int_\Omega \langle B^{-1} F_\epsilon, \mathcal{E} \rangle dx = 2 \int_\Omega \langle \mathscr{A}^{-1} \Lambda^{\frac{1}{2}} F_\epsilon, \Lambda^{\frac{1}{2}} \mathcal{E} \rangle dx \\
&\leq 2 \int_\Omega \left| \mathscr{A}^{-1} \right| \left| \Lambda^{\frac{1}{2}} F_\epsilon \right| \left| \Lambda^{\frac{1}{2}} \mathcal{E} \right| dx,
\end{aligned}$$

where the matrix D is defined by (1.11) and

$$\mathcal{E} = (\epsilon^1, \epsilon^2, \cdots, \epsilon^n)^T, \quad F_\epsilon = \left(\widetilde{f}_u^1 \epsilon^1, \widetilde{f}_u^2 \epsilon^2, \cdots, \widetilde{f}_u^n \epsilon^n \right)^T.$$

According to Lemmas 5.1, 5.2, Cauchy-Schwarz inequality and (5.4), we get

$$\begin{aligned}
\|\epsilon^n\|^2 - \|\epsilon^0\|^2 &\leq 2\gamma^{-1} \int_\Omega \left| \Lambda^{\frac{1}{2}} F_\epsilon \right| \left| \Lambda^{\frac{1}{2}} \mathcal{E} \right| dx \\
&\leq 2\gamma^{-1} \sqrt{\int_\Omega \left| \Lambda^{\frac{1}{2}} F_\epsilon \right|^2 dx} \sqrt{\int_\Omega \left| \Lambda^{\frac{1}{2}} \mathcal{E} \right|^2 dx} \\
&= 2\gamma^{-1} \sqrt{\int_\Omega \sum_{k=1}^{n} \tau_k \left(\widetilde{f}_u^k \epsilon^k \right)^2 dx} \sqrt{\int_\Omega \sum_{k=1}^{n} \tau_k (\epsilon^k)^2 dx} \\
&\leq 2\gamma^{-1} \widetilde{c} \int_\Omega \sum_{k=1}^{n} \tau_k (\epsilon^k)^2 dx = 2\gamma^{-1} \widetilde{c} \sum_{k=1}^{n} \tau_k \|\epsilon^k\|^2, \quad n \geq 1.
\end{aligned}$$

Choosing some integer n_1 $(0 \leq n_1 \leq n)$ such that $\|\epsilon^{n_1}\| = \max_{0 \leq k \leq n} \|\epsilon^k\|$. Taking $n := n_1$ in the above inequality, we get

$$\|\epsilon^n\| \leq \|\epsilon^0\| + 2\gamma^{-1} \widetilde{c} \sum_{k=1}^{n} \tau_k \|\epsilon^k\|, \quad n \geq 1.$$

Using the discrete Grönwall's inequality in Lemma 5.4 and for sufficiently small step-sizes τ_n (namely, $2\gamma^{-1} \widetilde{c} \tau_n < 1/2$), we get

$$\|\epsilon^n\| \leq 2 \exp\left(4\gamma^{-1} \widetilde{c} t_{n-1} \right) \|\epsilon^0\|, \quad n \geq 1.$$

The proof is complete. □

5.2. Convergence analysis

We are now at the stage to show the L^2 norm convergence analysis. We first consider the consistency error of the variable steps BDF3 scheme (1.7).

Lemma 5.5. *For the consistency error $\eta^j := D_3u(t_j) - \partial_t u(t_j)$ for $j \geq 1$, it holds that*

$$\|\eta^1\| \leq \int_0^{t_1} \|\partial_{tt}u\|dt, \quad \|\eta^2\| \leq 2\tau_2 \int_{t_1}^{t_2} \|\partial_{ttt}u\| + \frac{1}{2}\tau_1 \int_0^{t_1} \|\partial_{ttt}u\|,$$
$$\|\eta^j\| \leq C\left(\tau_j^2 \int_{t_{j-1}}^{t_j} \|\partial_{tttt}u\|dt + \tau_{j-1}^2 \int_{t_{j-2}}^{t_{j-1}} \|\partial_{tttt}u\|dt + \tau_{j-2}^2 \int_{t_{j-3}}^{t_{j-2}} \|\partial_{tttt}u\|dt\right), \quad j \geq 3.$$

Proof. For simplicity, denote

$$G_3^j = \int_{t_{j-1}}^{t_j} \|\partial_{ttt}u\|dt, \quad G_4^j = \int_{t_{j-1}}^{t_j} \|\partial_{tttt}u\|dt, \quad j \geq 1.$$

For the cases of $j = 1$ and $j = 2$, according to [7, Lemma 4.1], we have

$$\begin{aligned}
\|\eta^1\| &\leq \int_0^{t_1} \|\partial_{tt}u\|dt, \\
\|\eta^2\| &\leq \frac{1+2r_2}{1+r_2}\tau_2 G_3^2 + \frac{r_2}{2(1+r_2)}\tau_1 G_3^1 \\
&\leq 2\tau_2 \int_{t_1}^{t_2} \|\partial_{ttt}u\| + \frac{1}{2}\tau_1 \int_0^{t_1} \|\partial_{ttt}u\|.
\end{aligned}$$

For the case of $j \geq 3$, by using the Taylor's expansion formula, it yields

$$\begin{aligned}
\eta^j =& \frac{b_1^{(j)} - b_0^{(j)}}{6} \int_{t_{j-1}}^{t_j} (t - t_{j-1})^3 \partial_{tttt}u dt \\
&+ \frac{b_2^{(j)} - b_1^{(j)}}{6} \int_{t_{j-2}}^{t_j} (t - t_{j-2})^3 \partial_{tttt}u dt \\
&- \frac{b_2^{(j)}}{6} \int_{t_{j-3}}^{t_j} (t - t_{j-3})^3 \partial_{tttt}u dt.
\end{aligned}$$

According to (1.5), the consistency error is bounded by

$$\begin{aligned}
\|\eta^j\| &\leq C\big(b_0^{(j)}\tau_j^3 G_4^j - b_1^{(j)}\tau_{j-1}^3 G_4^{j-1} + b_2^{(j)}\tau_{j-2}^3 G_4^{j-2}\big) \\
&\leq C\left(\tau_j^2 \int_{t_{j-1}}^{t_j} \|\partial_{tttt}u\|dt + \tau_{j-1}^2 \int_{t_{j-2}}^{t_{j-1}} \|\partial_{tttt}u\|dt + \tau_{j-2}^2 \int_{t_{j-3}}^{t_{j-2}} \|\partial_{tttt}u\|dt\right).
\end{aligned}$$

The proof is complete. □

Theorem 5.2. *Let $u(t_n)$ and u^n be the solution of* (1.1) *and the* BDF3 *scheme* (1.7)*, respectively. Then the following error estimate holds for $1 \leq n \leq N$:*

$$
\begin{aligned}
&\|u(t_n)-u^n\|\\
&\leq C\Bigg(\tau_1^{\frac{1}{2}}\int_0^{t_1}\|\partial_{tt}u\|dt+\tau_2^{\frac{3}{2}}\int_{t_1}^{t_2}\|\partial_{ttt}u\|+\tau_1\tau_2^{\frac{1}{2}}\int_0^{t_1}\|\partial_{ttt}u\|\\
&\qquad+\sqrt{\sum_{k=3}^{n}\tau_k\left(\tau_k^2\int_{t_{k-1}}^{t_k}\|\partial_{tttt}u\|dt+\tau_{k-1}^2\int_{t_{k-2}}^{t_{k-1}}\|\partial_{tttt}u\|dt+\tau_{k-2}^2\int_{t_{k-3}}^{t_{k-2}}\|\partial_{tttt}u\|dt\right)^2}\Bigg).
\end{aligned}
$$

Proof. Let $e^n := u(t_n) - u^n$ be the error function with $e^0 = 0$. From (1.1) and (1.7), we have the following error equation:

$$D_3e^j - \varepsilon^2\Delta e^j = f(u^j) - f\big(u(t_j)\big) + \eta^j = f_u^j e^j + \eta^j, \quad j \geq 1, \tag{5.6}$$

where

$$f_u^j = 1 - (u^j)^2 - u^j u(t_j) - \big(u(t_j)\big)^2, \quad \eta^j = D_3u(t_j) - \partial_t u(t_j).$$

The energy dissipation law (1.3) of the Allen-Cahn equation (1.1) shows that

$$E\big(u(t_n)\big) \leq E\big(u(t_0)\big).$$

From the formulation (1.2), it is easy to check that $\|u(t_n)\|_{H^1}$ can be bounded by a time-independent constant c_2. Note that the solution estimates in Lemma 4.1 and $H^1 \subseteq L^\infty$, we have

$$
\begin{aligned}
\big\|f_u^j\big\|_{L^\infty} &\leq 1 + \|u^j\|_{L^\infty}^2 + \|u^j\|_{L^\infty}\|u(t_j)\|_{L^\infty} + \|u(t_j)\|_{L^\infty}^2\\
&\leq 1 + c_\Omega^2\|u^j\|_{H^1}^2 + c_\Omega^2\|u^j\|_{H^1}\|u(t_j)\|_{H^1} + c_\Omega^2\|u(t_j)\|_{H^1}^2\\
&\leq 1 + c_\Omega^2 c_1^2 + c_\Omega^2 c_1 c_2 + c_\Omega^2 c_2^2 := c_3, \quad j \geq 1.
\end{aligned} \tag{5.7}
$$

Multiplying both sides of (5.6) by the DOC kernels $d_{k-j}^{(k)}$, and summing j from 1 to k, we derive by applying the Eq. (5.5)

$$\nabla_\tau e^k - \varepsilon^2\sum_{j=1}^{k} d_{k-j}^{(k)}\Delta e^j = \sum_{j=1}^{k} d_{k-j}^{(k)} f_u^j e^j + \sum_{j=1}^{k} d_{k-j}^{(k)}\eta^j, \quad k \geq 1.$$

Making the inner product of the above equality with e^k and summing the resulting equality from $k = 1$ to n, there exists

$$\sum_{k=1}^{n}\big(\nabla_\tau e^k, e^k\big) + \varepsilon^2\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}(\nabla e^j, \nabla e^k) = \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}\big(f_u^j e^j, e^k\big) + \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}(\eta^j, e^k).$$

For the first term on the left hand, we have

$$\sum_{k=1}^{n}\big(\nabla_\tau e^k, e^k\big) \geq \frac{1}{2}\sum_{k=1}^{n}\big(\|e^k\|^2 - \|e^{k-1}\|^2\big) = \frac{1}{2}\big(\|e^n\|^2 - \|e^0\|^2\big),$$

where the inequality $2a(a-b) \geq a^2 - b^2$ has been used.

For the second term on the left hand, using Lemma 5.3, we obtain

$$\varepsilon^2 \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}(\nabla e^j, \nabla e^k) \geq 0.$$

From the above estimates, (1.11), Lemma 5.1, discrete Cauchy-Schwarz inequality and (3.1), it yields

$$\begin{aligned}
\|e^n\|^2 - \|e^0\|^2 &\leq 2\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}\big(f_u^j e^j, e^k\big) + 2\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}(\eta^j, e^k)\\
&= 2\int_\Omega E^T D F_e dx + 2\int_\Omega E^T D\Upsilon dx\\
&= 2\int_\Omega \langle DF_e, E\rangle dx + 2\int_\Omega \langle D\Upsilon, E\rangle dx\\
&= 2\int_\Omega \langle B^{-1}F_e, E\rangle dx + 2\int_\Omega \langle B^{-1}\Upsilon, E\rangle dx\\
&= 2\int_\Omega \big\langle \mathscr{A}^{-1}\Lambda^{\frac{1}{2}}F_e, \Lambda^{\frac{1}{2}}E\big\rangle dx + 2\int_\Omega \big\langle \mathscr{A}^{-1}\Lambda^{\frac{1}{2}}\Upsilon, \Lambda^{\frac{1}{2}}E\big\rangle dx\\
&\leq 2\int_\Omega \big|\mathscr{A}^{-1}\big|\big|\Lambda^{\frac{1}{2}}F_e\big|\big|\Lambda^{\frac{1}{2}}E\big| dx + 2\int_\Omega \big|\mathscr{A}^{-1}\big|\big|\Lambda^{\frac{1}{2}}\Upsilon\big|\big|\Lambda^{\frac{1}{2}}E\big| dx,
\end{aligned}$$

where

$$E = (e^1, e^2, \cdots, e^n)^T, \quad F_e = \big(f_u^1 e^1, f_u^2 e^2, \cdots, f_u^n e^n\big)^T, \quad \Upsilon = (\eta^1, \eta^2, \cdots, \eta^n)^T.$$

According to Lemmas 5.1, 5.2, Cauchy-Schwarz inequality and (5.7), we get

$$\begin{aligned}
\|e^n\|^2 - \|e^0\|^2 &\leq 2\gamma^{-1}\int_\Omega \big|\Lambda^{\frac{1}{2}}F_e\big|\big|\Lambda^{\frac{1}{2}}E\big| dx + 2\gamma^{-1}\int_\Omega \big|\Lambda^{\frac{1}{2}}\Upsilon\big|\big|\Lambda^{\frac{1}{2}}E\big| dx\\
&\leq 2\gamma^{-1}\left(\sqrt{\int_\Omega \big|\Lambda^{\frac{1}{2}}F_e\big|^2 dx} + \sqrt{\int_\Omega \big|\Lambda^{\frac{1}{2}}\Upsilon\big|^2 dx}\right)\sqrt{\int_\Omega \big|\Lambda^{\frac{1}{2}}E\big|^2 dx}\\
&= 2\gamma^{-1}\left(\sqrt{\int_\Omega \sum_{k=1}^{n}\tau_k\big(f_u^k e^k\big)^2 dx} + \sqrt{\int_\Omega \sum_{k=1}^{n}\tau_k(\eta^k)^2 dx}\right)\sqrt{\int_\Omega \sum_{k=1}^{n}\tau_k(e^k)^2 dx}\\
&\leq 2\gamma^{-1}c_3\sum_{k=1}^{n}\tau_k\|e^k\|^2 + 2\gamma^{-1}\sqrt{\sum_{k=1}^{n}\tau_k\|\eta^k\|^2}\sqrt{\sum_{k=1}^{n}\tau_k\|e^k\|^2}, \quad n\geq 1.
\end{aligned}$$

Taking some integer n_2 $(0 \leq n_2 \leq n)$ such that $\|e^{n_2}\| = \max_{0\leq k\leq n}\|e^k\|$. Setting $n := n_2$ in the above inequality, we get

$$\|e^n\| \leq \|e^0\| + 2\gamma^{-1}c_3\sum_{k=1}^{n}\tau_k\|e^k\| + 2\gamma^{-1}\sqrt{\sum_{k=1}^{n}\tau_k\|\eta^k\|^2}, \quad n\geq 1.$$

Using the discrete Grönwall's inequality in Lemma 5.4 and for sufficiently small step-sizes τ_n (namely, $2\gamma^{-1}c_3\tau_n < 1/2$), we get

$$\|e^n\| \leq 4\gamma^{-1}\exp\big(4\gamma^{-1}c_3 t_{n-1}\big)\sqrt{\sum_{k=1}^{n}\tau_k\|\eta^k\|^2}, \quad n\geq 1.$$

The desired result follows by Lemma 5.5. □

Remark 5.1. The corresponding theories can be extended to the high-dimensional case when the general nonlinear function $f(u)$ is Lipschitz continuous.

6. Numerical Examples

In this section, we provide some details on the numerical implementations and present several numerical examples to confirm our theoretical statements. For the variable steps BDF3 scheme (1.7) for the Allen-Cahn equation, we perform a simple Newton-type iteration at each time level with a tolerance 10^{-10}. We always choose the solution at the previous level as the initial value of Newton iteration. In space, we discretize by the spectral collocation method at Chebyshev-Gauss-Lobatto points [1, 20]

$$u_I^n(x,y)=\sum_{i=0}^{M_x}\sum_{j=0}^{M_y}u_{ij}^n\ell_i(x)\ell_j(y),\quad \ell_i(x)=\prod_{\substack{j=0\\ j\neq i}}^{M_x}\frac{x-x_j}{x_i-x_j},$$

where $u_{ij}^n:=u_I^n(x_i,y_j)$. Here, $-1=x_0<x_1<\cdots<x_{M_x}=1$ and $-1=y_0<y_1<\cdots<y_{M_y}=1$ are nodes of Lobatto quadrature rules.

Example 6.1. We numerically verify the theoretical results including convergence orders in the discrete L^2-norm. In order to investigate the temporal convergence rate, we fix $M_x=M_y=20$, the spatial error is negligible since the spectral collocation method converges exponentially, see, e.g. [20, Theorem 4.4].

The initial value and the forcing term are chosen such that the exact solution of Eq. (1.1) is

$$u(x,y,t)=(t^4+1)\cos(\pi x)\cos(\pi y),\quad -1\leqslant x,y\leqslant 1,\quad 0\leqslant t\leqslant 1$$

with the (inhomogeneous) periodic boundary conditions

$$\begin{aligned}u(-1,y,t)&=u(1,y,t)=-(t^4+1)\cos(\pi y),\\ u(x,-1,t)&=u(x,1,t)=-\big(t^4+1\big)\cos(\pi x).\end{aligned}$$

Here, we consider two cases of the adjacent time-step ratios r_k.

Case I: $r_{2k}=2$ for $1\le k\le N/2$, and $r_{2k-1}=1/2$ for $2\le k\le N/2$.

Case II: The arbitrary meshes with random time-steps $\tau_k=T\sigma_k/S$ for $1\le k\le N$, where $S=\sum_{k=1}^N\sigma_k$ and $\sigma_k\in(0,1)$ are random numbers subject to the uniform distribution [7, 18].

As observed in Table 6.1, the variable steps BDF3 scheme (1.7) achieves the third-order accuracy even when the chosen step ratios are larger than expected requirement $r_n=\tau_n/\tau_{n-1}\le 1.405$. The same phenomena are also observed for variable steps BDF2 method in [16]. The numerical experiments indicate that the BDF3 method is much more robust with respect to the step-size variations than previous theoretical predictions. In fact, the improved condition $r_n=\tau_n/\tau_{n-1}\le 1.405$ is still a sufficient conditions for third-order convergence, since it just ensures the positive definiteness of the matrix B in (1.11) or the scaled matrix A in (2.2).

Table 6.1: The discrete L^2-norm errors and numerical convergence orders.

Case I						
N	$\varepsilon = 0.1$	Rate	$\varepsilon = 0.02$	Rate	$\max r_k$	$\min r_k$
80	6.7445e-06		9.5503e-06		2	1/2
160	8.4200e-07	3.0018	1.1924e-06	3.0016	2	1/2
320	1.0518e-07	3.0009	1.4896e-07	3.0009	2	1/2
640	1.3142e-08	3.0007	1.8613e-08	3.0006	2	1/2
Case II						
N	$\varepsilon = 0.1$	Rate	$\varepsilon = 0.02$	Rate	$\max r_k$	$\min r_k$
80	9.3468e-06		1.3314e-05		48.8928	0.0121
160	1.1953e-06	2.9671	1.7255e-06	2.9478	76.0331	0.0121
320	1.6040e-07	2.8976	2.2458e-07	2.9418	76.0331	0.0061
640	1.9113e-08	3.0691	2.7307e-08	3.0399	76.0331	0.0061

Example 6.2. We next consider the Allen-Cahn model (1.1) with the diffusion coefficient $\varepsilon = 0.02$. The variable steps BDF3 scheme (1.7) is applied to simulate the merging of four bubbles with an initial condition

$$u_0(x,y) = -\tanh\left(\frac{(x-0.3)^2+y^2-0.2^2}{\varepsilon}\right)\tanh\left(\frac{(x+0.3)^2+y^2-0.2^2}{\varepsilon}\right) \times\tanh\left(\frac{x^2+(y-0.3)^2-0.2^2}{\varepsilon}\right)\tanh\left(\frac{x^2+(y+0.3)^2-0.2^2}{\varepsilon}\right).$$

The computational domain is $\Omega = (-1,1)^2$ with $M_x = M_y = 70$. Here the (inhomogeneous) periodic boundary conditions are

$$u(-1,y,t) = u(1,y,t) = -1,$$
$$u(x,-1,t) = u(x,1,t) = -1.$$

We use the arbitrary meshes with random time-steps $\tau_k = T\sigma_k/S$ for $1 \le k \le N$. Here $S = \sum_{k=1}^{N}\sigma_k, T = 100, N = 10000$ and $\sigma_k \in (0,1)$ are random numbers subject to the uniform distribution. The time evolution of the phase variable is summarized in Fig. 6.1. We observe that the initial separated four bubbles gradually coalesce into a single bubble.

Example 6.3. We finally consider the coarsening dynamics of the Allen-Cahn model (1.1) with the diffusion coefficient $\varepsilon = 0.02$. We choose a random initial condition $u_0(x,y) = -0.5 + \text{rand}(x,y)$. The computational domain is $\Omega = (-1,1)^2$ with the (inhomogeneous) periodic boundary conditions

$$u(-1,y,t) = u(1,y,t) = -1,$$
$$u(x,-1,t) = u(x,1,t) = -1.$$

We first investigate the effect of the arbitrary meshes with random time-step size on the maximum norm and discrete energy. The numerical results are shown with $T = 20, N = 20000$, $M_x = M_y = 5$ in Fig. 6.2. We observe that the maximum values of the numerical solutions are bounded by 1 and the discrete energy decays monotonically, which satisfied the maximum bound principle [16] and energy decay for the Allen-Cahn equation.

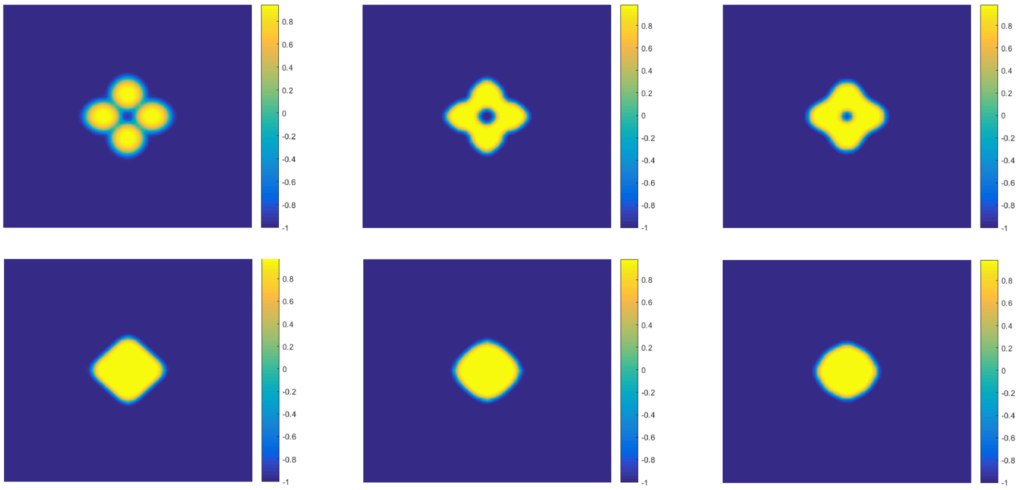

Fig. 6.1. Solution of the Allen-Cahn equation using the arbitrary meshes at $t = 0, 10, 20, 40, 70, 100$ (from left to right), respectively.

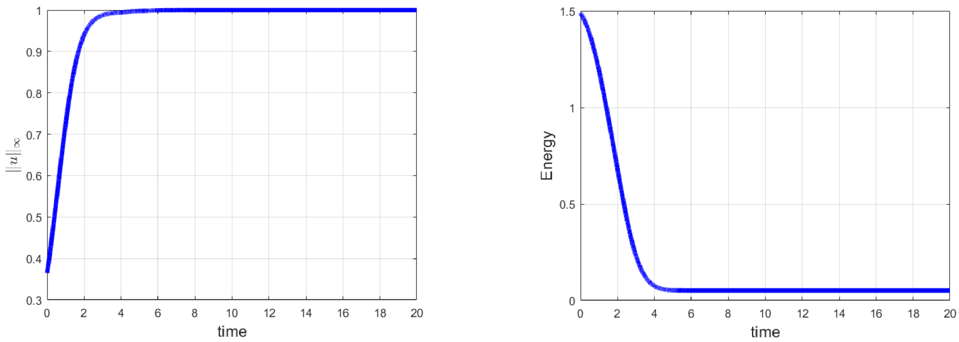

Fig. 6.2. Illustration of the maximum bound principle and energy decay for Allen-Cahn equation, left and right, respectively.

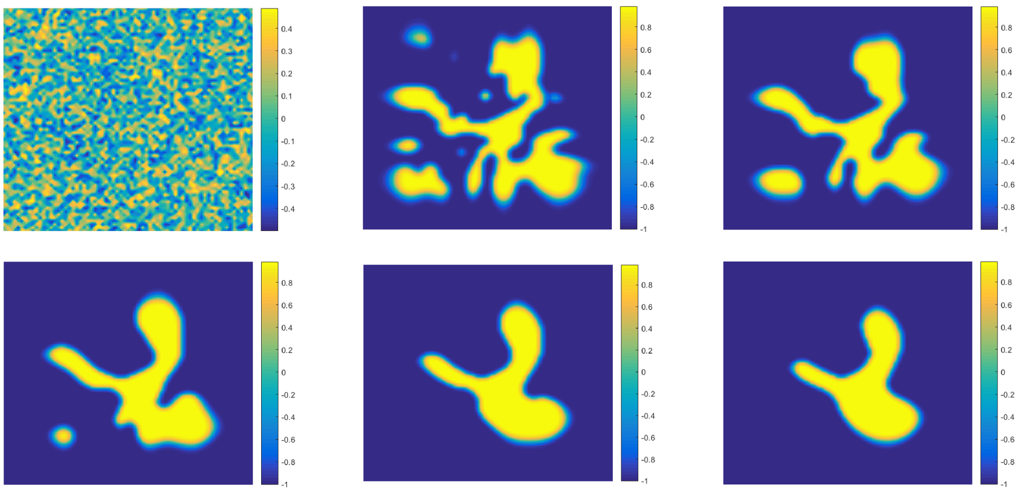

Fig. 6.3. Solution of coarsening dynamics of the Allen-Cahn equation using the arbitrary meshes at $t = 0, 10, 20, 40, 70, 100$ (from left to right), respectively.

We finally investigate the coarsening dynamics of the Allen-Cahn model (1.1) by using the arbitrary meshes with random time-step size until $T = 100, N = 10000, M_x = M_y = 70$. In Fig. 6.3, we observe that the microstructure contains a large number of grains at $t = 0$. As time evolves, the coarsening dynamics through migration of the phase boundaries, decomposition, and merging procedure can be observed. Also, the number of grains becomes smaller with time. It should be noted that we shall adopt an adaptive time-stepping strategy in [11,16] to choose the time-step size for the above numerical experiments.

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