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THE WEIGHTED AND SHIFTED TWO-STEP BDF METHOD FOR ALLEN-CAHN EQUATION ON VARIABLE GRIDS

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Abstract. The weighted and shifted seven-step BDF method is proposed by the authors [Akrivis, Chen, and Yu, IMA. Numer. Anal., DOI:10.1093/imanum/drae089] for parabolic equation on uniform meshes. In this paper, we study the weighted and shifted two-step BDF method (WSBDF2) for the Allen-Cahn equation on variable grids. In order to preserve a modified energy dissipation law at the discrete level, a novel technique is designed to deal with the nonlinear term. The stability and convergence analysis of the WSBDF2 method are rigorously proved by the energy method under the adjacent time-step ratios $r_s \geq 4.8645$. Finally, numerical experiments are implemented to illustrate the theoretical results. The proposed approach is applicable for the Cahn-Hilliard equation.

Key words. Weighted and shifted two-step BDF method, variable step size, Allen-Cahn equation, stability and convergence analysis.

1. Introduction

The objective of this paper is to provide a rigorous stability and convergence analysis on variable grids for solving the Allen-Cahn equation [1]

$$\partial_t u - \varepsilon^2 \Delta u + f(u) = 0, \quad (x,t) \in \Omega \times (0,T] \tag{1}$$

with the initial condition $u(0) = u_0$ and periodic boundary conditions. Here, the nonlinear bulk force is defined as $f(u) = F'(u) = u^3 - u$, and the parameter $\varepsilon > 0$ denotes the interfacial width. The Allen-Cahn equation can be regarded as an L^2-gradient flow of the following free energy functional:

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

In other words, the Allen-Cahn equation (1) satisfies the energy dissipation law:

$$\frac{dE[u]}{dt} = -\int_\Omega |\partial_t u|^2 \, dx \leq 0. \tag{3}$$

Let $N \in \mathbb{N}$ and consider 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 $\{v^n\}_{n=0}^N$, we denote

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

For $k = 1, 2$, let $\Pi_{n,k} v$ denote the interpolating polynomial of a function v over $k+1$ nodes $t_{n-k}, \cdots, t_{n-1}$ and t_n. Taking $v^n = v(t_n)$, and using the Lagrange interpolation, the one-step BDF formula yields $D_1 v^n := (\Pi_{n,1} v)'(t) = \nabla_\tau v^n / \tau_n$ for $n \geq 1$, and the two-step BDF formula reads

$$D_2 v^n = \left(\Pi_{n,2} v\right)'(t_n) = \frac{1 + 2r_n}{\tau_n(1 + r_n)} \nabla_\tau v^n - \frac{r_n^2}{\tau_n(1 + r_n)} \nabla_\tau v^{n-1}, \quad n \geq 2,$$

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where the adjacent time-step ratios are defined by

$$r_1 := 0, \quad r_n := \frac{\tau_n}{\tau_{n-1}}, \quad n \geq 2.$$

Similarly, we construct the shifted two-step BDF formula as follows:

$$\widetilde{D}_2 v^n = (\Pi_{n,2} v)'(t_{n-1}) = \frac{1}{\tau_n(1+r_n)} \nabla_\tau v^n + \frac{r_n^2}{\tau_n(1+r_n)} \nabla_\tau v^{n-1}, \quad n \geq 2.$$

Thus, the weighted and shifted two-step BDF (WSBDF2) formula is defined by

$$\mathcal{D}_2 v^n := \theta D_2 v^n + (1-\theta)\, \widetilde{D}_2 v^n, \quad n \geq 2,$$

i.e.,

$$\mathcal{D}_2 v^n = \frac{1+2\theta r_n}{\tau_n(1+r_n)} \nabla_\tau v^n + \frac{(1-2\theta) r_n^2}{\tau_n(1+r_n)} \nabla_\tau v^{n-1}, \quad \theta \in [1/2, 1]\,. \tag{4}$$

It is noted that the WSBDF2 formula (4) is a flexible form between the Crank-Nicolson ($\theta = 1/2$) and the two-step BDF ($\theta = 1$) approximations for the discretization of the first order derivative $\partial_t u$ on nonuniform meshes. The WSBDF2 formula (4) coincides with the implicit-explicit multistep method of order 2 in [21]. However, the construction techniques are significantly different. In [21], the coefficients are derived from order conditions. In contrast, the WSBDF2 formula (4) is constructed by the weighted and shifted technique, which is simpler and more flexible to design the high-order methods, such as the weighted and shifted seven-step BDF method [3].

Since the WSBDF2 formula requires two starting values, we use the weighted and shifted one-step BDF formula to compute first-level solution u^1 by

$$\mathcal{D}_2 v^1 := \theta(\Pi_{1,1} v)'(t_1) + (1-\theta)\, (\Pi_{1,1} v)'(t_0) = \nabla_\tau v^1 / \tau_1. \tag{5}$$

We recursively define a sequence of approximations u^n to the nodal values $u(t_n)$ of the exact solution by the WSBDF2 method,

$$\mathcal{D}_2 u^n - \varepsilon^2 \left(\theta \Delta u^n + (1-\theta)\Delta u^{n-1}\right) + H(u^n) = 0, \quad n \geq 1, \tag{6}$$

where the initial data is $u^0 = u_0$, and the nonlinear term $H(u^n)$ is constructed by

$$\begin{aligned} H(u^n) &= \theta f(u^n) + \left(1-\theta\right) f(u^{n-1}) - \frac{\theta}{2}\left(u^n + u^{n-1}\right)\left(u^n - u^{n-1}\right)^2 \\ &= \frac{\theta}{2}\left((u^n)^3 + (u^n)^2 u^{n-1} + u^n (u^{n-1})^2 - (u^{n-1})^3\right) \\ &\quad - \theta u^n + (1-\theta)\left((u^{n-1})^3 - u^{n-1}\right). \end{aligned} \tag{7}$$

The WSBDF2 formula (4) can be viewed as a discrete convolution summation:

$$\mathcal{D}_2 v^n = \sum_{k=1}^{n} b_{n-k}^{(n)} \nabla_\tau v^k, \quad n \geq 1, \tag{8}$$

where the discrete convolution kernels $b_{n-k}^{(n)}$ are defined by $b_0^{(1)} = 1/\tau_1$, and for $n \geq 2$,

$$b_0^{(n)} := \frac{1+2\theta r_n}{\tau_n(1+r_n)}, \quad b_1^{(n)} := \frac{(1-2\theta) r_n^2}{\tau_n(1+r_n)} \quad \text{and} \quad b_j^{(n)} := 0, \quad 2 \leq j \leq n-1. \tag{9}$$

The discrete orthogonal convolution (DOC) kernels $d_{n-k}^{(n)}$ are defined by

(10)

$$d_0^{(n)} := \frac{1}{b_0^{(n)}}, \quad d_{n-k}^{(n)} := -\frac{1}{b_0^{(k)}} \sum_{j=k+1}^{n} d_{n-j}^{(n)} b_{j-k}^{(j)} = -\frac{b_1^{(k+1)}}{b_0^{(k)}} d_{n-k-1}^{(n)}, \quad 1 \le k \le n-1.$$

Obviously, the DOC kernels $d_{n-k}^{(n)}$ satisfy the discrete orthogonal identity:

$$\sum_{j=k}^{n} d_{n-j}^{(n)} b_{j-k}^{(j)} \equiv \delta_{nk}, \quad 1 \le k \le n. \tag{11}$$

For convenience, we introduce the following matrices:

$$B := \begin{pmatrix} b_0^{(1)} & & & \\ b_1^{(2)} & b_0^{(2)} & & \\ & \ddots & \ddots & \\ & & b_1^{(n)} & b_0^{(n)} \end{pmatrix} \quad \text{and} \quad D := \begin{pmatrix} d_0^{(1)} & & & \\ d_1^{(2)} & d_0^{(2)} & & \\ \vdots & \vdots & \ddots & \\ d_{n-1}^{(n)} & d_{n-2}^{(n)} & \cdots & d_0^{(n)} \end{pmatrix}, \tag{12}$$

where the discrete convolution kernels $b_{n-k}^{(n)}$ and the DOC kernels $d_{n-k}^{(n)}$ are defined in (9) and (10), respectively. From the discrete orthogonal identity (11), there exists

$$D = B^{-1}. \tag{13}$$

Variable steps implicit-explicit multistep methods for PDEs have been presented in [6, 21], where the zero-stability is studied for ODEs. However, the stability analysis for PDEs still remains an open problem, which motivates us to consider the work. Nowadays, many researchers focus on the numerical analysis for parabolic problems with variable steps. The variable two-step BDF method for ODEs is zero-stable if the adjacent time-step ratios $r_n < 1 + \sqrt{2}$ in [10, 13], also see [14, p. 405]. Standard stability estimates have been proved by Becker [7] and Emmrich [12] for parabolic equation under the adjacent time-step ratios $r_n \le 1.8685$ and 1.9104, respectively. Recently, the standard stability is established by the authors for the adjacent time-step ratios up to 1.9398 in [2]. The adaptive two-step BDF method for the linear diffusion equation is considered under $r_n \le (3+\sqrt{17})/2 \approx 3.561$ in [16]. Later on, the adjacent time-step ratio has been extended to $r_n \le 4.8645$ in [17, 23]. Using the Crank-Nicolson reconstructions technique, a posteriori error estimate has been obtained for the parabolic equation with variable steps in [5]. The general linear second-order schemes are considered on uniform meshes for thermodynamical consistent models [24] and phase field models [8]. In this work, we present the WSBDF2 method on variable grids for the Allen-Cahn equation, where a novel technique is proposed for handling the nonlinear term. The stability and convergence are rigorously established by the energy method under the adjacent time-step ratios $r_s \ge 4.8645$ in (17), which fill in the gap of the theory for PDEs in [21].

The proposed WSBDF2 method can be applied to the Cahn-Hilliard equation [8, 17], since the Allen-Cahn equation and Cahn-Hilliard equation are the L^2 and H^{-1} gradient flows of the free energy functional (2), respectively.

An outline of the paper is organized as follows: In the next section, the upper bound for adjacent time-step ratios is proved, including the suboptimal ratios r_p and optimal ratios r_s, ensuring that the discrete convolution kernels $b_{n-k}^{(n)}$ are positive semi-definite, which plays a crucial role in the stability and convergence analysis.

In Section 3, the unique solvability and discrete energy stability are demonstrated under the adjacent time-step ratios r_s. The stability and convergence are rigorously established by the energy method in Section 4 and 5, respectively. In Section 6, numerical examples are carried out to validate the theoretical results. Finally, the paper concludes with some remarks.

2. Upper bound for the adjacent time-step ratios

We establish the upper bound for the adjacent time-step ratios, ensuring that the discrete convolution kernels $b_{n-k}^{(n)}$ are positive semi-definite, which is vital to the stability and convergence analysis.

Lemma 2.1. [18, p. 28] *A real matrix L of order n is positive definite if and only if its symmetric part $H = \frac{L+L^T}{2}$ is positive definite.*

Lemma 2.2. [18, p. 29] *(Sylvester criterion) Let $P \in \mathbb{R}^{n\times n}$ be a symmetric matrix. Then, P is positive definite if and only if the dominant principal minors of P are all positive.*

Lemma 2.3. *Let the adjacent time-step ratios r_n satisfy $0 < r_n \le r_p$ in (16) for $2 \le n \le N$. Then, for any real sequence $\{w_k\}_{k=1}^n$, it holds that*

$$\sum_{k=1}^{n} w_k \sum_{j=1}^{k} b_{k-j}^{(k)} w_j \ge 0, \quad n \ge 1.$$

Proof. We can verify that

$$\sum_{k=1}^{n} w_k \sum_{j=1}^{k} b_{k-j}^{(k)} w_j = W^T B W, \quad n \ge 1,$$

where $W = (w_1, w_2, \cdots, w_n)^T$ and the matrix B is defined in (12). We introduce the symmetric tridiagonal matrix $\widetilde{B} := B + B^T = (\widetilde{b}_{ij})$ with entries

$$\widetilde{b}_{i,j} = \begin{cases} 2b_0^{(i)}, & 1 \le i = j \le n, \\ b_1^{(i)}, & j = i-1, \quad i = 2, \dots, n, \\ b_1^{(j)}, & j = i+1, \quad i = 1, \dots, n-1, \end{cases}$$

and all other entries equal zero.

In order to prove that matrix B is positive definite, it suffices to prove that the matrix $\widetilde{B}$ is positive definite.

By linear transformation, the matrix $\widetilde{B}$ can be transformed into an upper triangular matrix $L = (\ell_{ij})$ with entries

$$\ell_{i,j} = \begin{cases} 2b_0^{(1)}, & i = j = 1, \\ 2b_0^{(i)} - \dfrac{1}{\ell_{i-1,i-1}} \left(b_1^{(i)}\right)^2, & 2 \le i = j \le n, \\ b_1^{(j)}, & j = i+1, \quad i = 1, \dots, n-1, \end{cases} \tag{14}$$

and all other entries equal zero. With this notation, we have $\ell_{1,1} = 2b_0^{(1)} = \frac{2}{\tau_1}$. In the following, we use the mathematical induction to prove

$$\ell_{i,i} \ge \frac{2}{\tau_i}, \quad 2 \le i \le n. \tag{15}$$

For $i=2$, based on (14) and (9), we obtain

$$\begin{aligned}\ell_{2,2} &= 2b_0^{(2)} - \frac{1}{\ell_{1,1}}\left(b_1^{(2)}\right)^2 = \frac{2\left(1+2\theta r_2\right)}{\tau_2\left(1+r_2\right)} - \frac{\tau_1\left(1-2\theta\right)^2 r_2^4}{2\tau_2^2\left(1+r_2\right)^2} \\ &= \frac{2\left(1+2\theta r_2\right)}{\tau_2(1+r_2)} - \frac{(1-2\theta)^2 r_2^3}{2\tau_2(1+r_2)^2} = \frac{4\left(1+2\theta r_2\right)\left(1+r_2\right) - (1-2\theta)^2 r_2^3}{2\tau_2(1+r_2)^2} \\ &= \frac{4(1+r_2)^2 - 4(1+r_2)^2 + 4\left(1+2\theta r_2\right)\left(1+r_2\right) - (1-2\theta)^2 r_2^3}{2\tau_2(1+r_2)^2} \\ &= \frac{2}{\tau_2} + \frac{-4\left(1+r_2\right)^2 + 4\left(1+2\theta r_2\right)\left(1+r_2\right) - \left(1-2\theta\right)^2 r_2^3}{2\tau_2(1+r_2)^2}.\end{aligned}$$

If the time-step ratios $0 < r_n \le r_p$, the suboptimal adjacent time-step ratios

$$r_p = \frac{2+2\sqrt{2\theta}}{2\theta-1} \tag{16}$$

is the positive root of equation $\left(1-2\theta\right) r_p^2 + 4r_p + 4 = 0$, we get

$$\begin{aligned}&-4\left(1+r_2\right)^2 + 4\left(1+2\theta r_2\right)\left(1+r_2\right) - \left(1-2\theta\right)^2 r_2^3 \\ &= \left(2\theta-1\right) r_2 \left(\left(1-2\theta\right) r_2^2 + 4r_2 + 4\right) \ge 0.\end{aligned}$$

Therefore, (15) is proved for $i=2$.

Suppose that (15) holds for all $2 \le i \le n-1$. Now we need to prove that it also holds for $i=n$. For $i=n$, according to (14), (9) and the induction hypothesis, we have

$$\begin{aligned}\ell_{n,n} &= 2b_0^{(n)} - \frac{1}{\ell_{n-1,n-1}}\left(b_1^{(n)}\right)^2 = \frac{2\left(1+2\theta r_n\right)}{\tau_n\left(1+r_n\right)} - \frac{\tau_{n-1}\left(1-2\theta\right)^2 r_n^4}{2\tau_n^2\left(1+r_n\right)^2} \\ &= \frac{2\left(1+2\theta r_n\right)}{\tau_n(1+r_n)} - \frac{(1-2\theta)^2 r_n^3}{2\tau_n(1+r_n)^2} = \frac{4\left(1+2\theta r_n\right)\left(1+r_n\right) - (1-2\theta)^2 r_n^3}{2\tau_n(1+r_n)^2} \\ &= \frac{4(1+r_n)^2 - 4(1+r_n)^2 + 4\left(1+2\theta r_n\right)\left(1+r_n\right) - (1-2\theta)^2 r_n^3}{2\tau_n(1+r_n)^2} \\ &= \frac{2}{\tau_n} + \frac{-4\left(1+r_n\right)^2 + 4\left(1+2\theta r_n\right)\left(1+r_n\right) - \left(1-2\theta\right)^2 r_n^3}{2\tau_n(1+r_n)^2}.\end{aligned}$$

Similarly, we have

$$\begin{aligned}&-4\left(1+r_n\right)^2 + 4\left(1+2\theta r_n\right)\left(1+r_n\right) - \left(1-2\theta\right)^2 r_n^3 \\ &= \left(2\theta-1\right) r_n \left(\left(1-2\theta\right) r_n^2 + 4r_n + 4\right) \ge 0, \quad 0 < r_n \le r_p.\end{aligned}$$

Therefore, (15) is proved for $i=n$.

According to (15), we know that the diagonal entries of the matrix L are positive, i.e., $\ell_{i,i} > 0,\ 1 \le i \le N$. Since the symmetric tridiagonal matrix $\widetilde{B}$ is transformed into the upper triangular matrix $L = (\ell_{ij})$ by linear transformation, we obtain $\det \widetilde{B}_{n\times n} = \det L_{n\times n} = \prod_{i=1}^{n} \ell_{i,i} > 0,\ n \ge 1$, which implies the dominant principal minors of $\widetilde{B}$ are all positive. Based on Lemma 2.2, the matrix $\widetilde{B}$ is positive definite. Hence, the matrix B is also positive definite by Lemma 2.1. □

According to the proof of Lemma 2.3, we obtain the suboptimal adjacent time-step ratios r_p in (16)

$$r_p = \frac{2+2\sqrt{2\theta}}{2\theta-1}.$$

Next, we proceed to provide the optimal adjacent time-step ratios r_s,

$$r_s = \frac{4\theta^2 - \sqrt[3]{-4\theta^2 E + 3(1-2\theta)^2 \frac{-F+\sqrt{G}}{2}} - \sqrt[3]{-4\theta^2 E + 3(1-2\theta)^2 \frac{-F-\sqrt{G}}{2}}}{3(1-2\theta)^2} \tag{17}$$

with

$$\begin{aligned} E &= 16\theta^4 + 48\theta^3 - 48\theta^2 + 12\theta, \\ F &= 16\theta^3 + 36\theta^2 - 36\theta + 9, \\ G &= 384\theta^5 + 912\theta^4 - 2496\theta^3 + 1944\theta^2 - 648\theta + 81, \end{aligned}$$

which is the positive root of the equation

$$(1-2\theta)^2 r_s^3 - 4\theta^2 r_s^2 - 4\theta r_s - 1 = 0. \tag{18}$$

The suboptimal and optimal adjacent time-step ratios, denoted as r_p (16) and r_s (17), respectively, are plotted with respect to θ, see Figure 1. It is observed that the ratios r_p and r_s are decreasing for $\theta \in [1/2, 1]$. Thus, $r_p \geq 2 + 2\sqrt{2}$ and $r_s \geq \frac{4 + \sqrt[3]{\frac{299 - 3\sqrt{177}}{2}} + \sqrt[3]{\frac{299 + 3\sqrt{177}}{2}}}{3} \approx 4.8645$ for $\theta \in [1/2, 1]$.

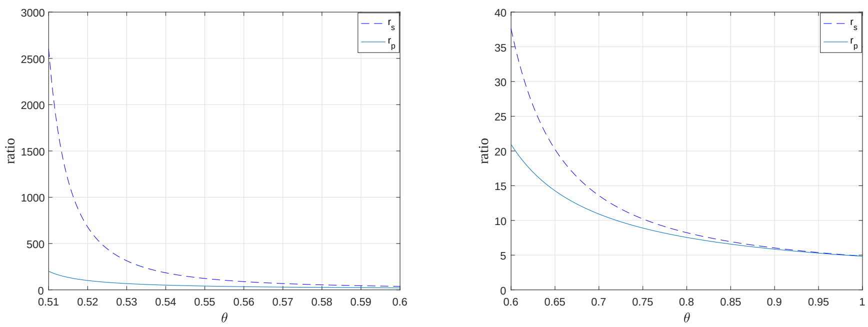

FIGURE 1. The graphs of ratios r_p (16) and r_s (17).

Lemma 2.4. *Let the adjacent time-step ratios r_n satisfy $0 < r_n \leq r_s$ in (17) for $2 \leq n \leq N$. Then, for any real sequence $\{\omega_k\}_{k=1}^n$, it holds that*

$$2\omega_k \sum_{j=1}^{k} b_{k-j}^{(k)} \omega_j \geq \frac{(2\theta-1) r_{k+1}^{3/2}}{1 + r_{k+1}} \frac{\omega_k^2}{\tau_k} - \frac{(2\theta-1) r_k^{3/2}}{1+r_k} \frac{\omega_{k-1}^2}{\tau_{k-1}} + h(r_k, r_{k+1}) \frac{\omega_k^2}{\tau_k}, \quad k \geq 2,$$

where

$$h(x,y) := \frac{2(1+2\theta x) + (1-2\theta)x^{3/2}}{1+x} - \frac{(2\theta-1) y^{3/2}}{1+y}, \quad 0 < x, y \leq r_s. \tag{19}$$

Then, the discrete convolution kernels $b_{n-k}^{(n)}$ defined in (9) are positive semi-definite,

$$\sum_{k=1}^{n} \omega_k \sum_{j=1}^{k} b_{k-j}^{(k)} \omega_j \geq 0, \quad n \geq 1.$$

Proof. Applying the inequality $2ab \le a^2+b^2$ and taking $u_k=\omega_k/\sqrt{\tau_k}$, we get

$$\begin{aligned}
2\omega_k\sum_{j=1}^{k} b_{k-j}^{(k)}\omega_j &= 2\tau_k b_0^{(k)} u_k^2 + 2\sqrt{\tau_k\tau_{k-1}}\, b_1^{(k)} u_k u_{k-1}\\
&\ge 2\tau_k b_0^{(k)} u_k^2 + \sqrt{\tau_k\tau_{k-1}}\, b_1^{(k)} \left(u_k^2+u_{k-1}^2\right)\\
&= \frac{2\left(1+2\theta r_k\right)+\left(1-2\theta\right) r_k^{3/2}}{1+r_k} u_k^2 - \frac{\left(2\theta-1\right) r_k^{3/2}}{1+r_k} u_{k-1}^2\\
&= \frac{\left(2\theta-1\right) r_{k+1}^{3/2}}{1+r_{k+1}}\frac{\omega_k^2}{\tau_k} - \frac{\left(2\theta-1\right) r_k^{3/2}}{1+r_k}\frac{\omega_{k-1}^2}{\tau_{k-1}}\\
&\quad + \left(\frac{2\left(1+2\theta r_k\right)+\left(1-2\theta\right) r_k^{3/2}}{1+r_k} - \frac{\left(2\theta-1\right) r_{k+1}^{3/2}}{1+r_{k+1}}\right)\frac{\omega_k^2}{\tau_k}, \quad k\ge 2.
\end{aligned}$$

It is easy to verify that $h(x,y)$ defined in (19) is increasing in $(0,1)$ and decreasing in $(1,r_s)$ with respect to x, and $h(x,y)$ is decreasing with respect to y. Then, we have

$$h(x,y)\ge \min\left\{h(0,r_s),h(r_s,r_s)\right\} = \frac{2\left(1+2\theta r_s+\left(1-2\theta\right) r_s^{3/2}\right)}{1+r_s} = 0,\ \ 0<x,y\le r_s,$$

where we have used the fact that r_s is the positive root of equation (18).

Thus it follows that

$$2\omega_k\sum_{j=1}^{k} b_{k-j}^{(k)}\omega_j \ge \frac{(2\theta-1)r_{k+1}^{3/2}}{1+r_{k+1}}\frac{\omega_k^2}{\tau_k} - \frac{(2\theta-1)r_k^{3/2}}{1+r_k}\frac{\omega_{k-1}^2}{\tau_{k-1}}, \quad 0<r_k\le r_s.$$

Therefore, we obtain

$$\begin{aligned}
2\sum_{k=1}^{n}\omega_k\sum_{j=1}^{k} b_{k-j}^{(k)}\omega_j &\ge \frac{2}{\tau_1}\omega_1^2 + \frac{(2\theta-1)r_{n+1}^{3/2}}{1+r_{n+1}}\frac{\omega_n^2}{\tau_n} - \frac{(2\theta-1)r_2^{3/2}}{1+r_2}\frac{\omega_1^2}{\tau_1}\\
&= \frac{(2\theta-1)r_{n+1}^{3/2}}{1+r_{n+1}}\frac{\omega_n^2}{\tau_n} + \frac{2+2r_2-(2\theta-1)r_2^{3/2}}{1+r_2}\frac{\omega_1^2}{\tau_1}\ge 0,
\end{aligned}$$

where we use

$$\frac{2+2r_2-(2\theta-1)r_2^{3/2}}{1+r_2} = \frac{1+2(1-\theta)r_2}{1+r_2} + \frac{1}{2}h(r_2,r_2)\ge 0.$$

In particular, (17) leads to $r_s = 4.8645365123$ if $\theta=1$ and $r_s\to\infty$ if $\theta=\frac{1}{2}$. □

Remark 2.1. From (14), we can check that $\ell_{1,1}=\frac{1}{\tau_1}\cdot l_1$ and $\ell_{k,k}=\frac{1}{\tau_k}\cdot l_k$ with

$$l_1=2,\quad l_k=\frac{2}{\left(1+r_k\right)^2}\left[\left(1+r_k\right)\left(1+2\theta r_k\right)-\frac{1}{2l_{k-1}}\left(2\theta-1\right)^2 r_k^3\right],\quad k\ge 2.$$

According to the proof of Lemma 2.4, we know that the matrix $\widetilde{B}$ is positive definite if and only if $l_k>0$. Figure 2 shows the optimal maximum ratios $r_s=4.8645$ for the variable two-step BDF method ($\theta=1$), since $l_k<0$ when $r_s=4.8646$. On the other hand, $l_k\equiv 2$ for the variable Crank-Nicolson method ($\theta=1/2$), which implies the ratio $r_s\to\infty$ (without restriction).

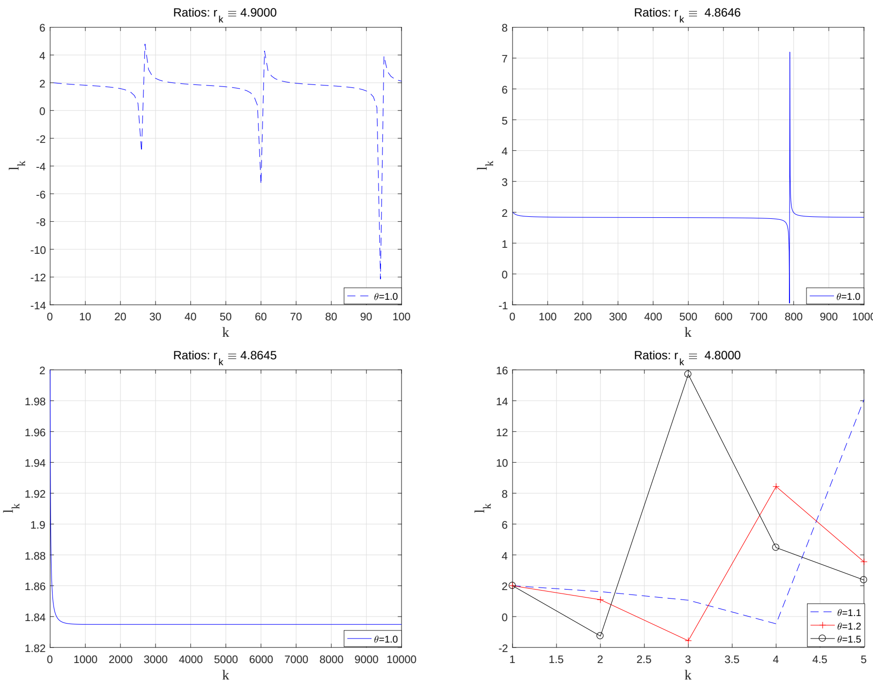

FIGURE 2. Simulations to maximum (constant) ratios r_s versus θ.

Lemma 2.5. *If the discrete convolution kernels $b^{(n)}_{n-k}$ defined in* (9) *are positive semi-definite, then the DOC kernels $d^{(n)}_{n-k}$ defined in* (10) *are also positive semi-definite. For any real sequence $\{w_k\}^n_{k=1}$, it holds that*

$$\sum_{k=1}^{n} w_k \sum_{j=1}^{k} d^{(k)}_{k-j} w_j \geq 0, \quad n \geq 1.$$

Proof. We can verify that

$$\sum_{k=1}^{n} w_k \sum_{j=1}^{k} d^{(k)}_{k-j} w_j = W^T D W, \quad n \geq 1,$$

where $W = (w_1, w_2, \cdots, w_n)^T$ and the matrix D is defined in (12).

According to Lemma 2.3 or Lemma 2.4, the matrix B is positive semi-definite. Let $\nu = BW \neq 0$. From (13), it yields

$$\nu^T D \nu = \nu^T B^{-1} \nu = W^T B^T B^{-1} BW = W^T B^T W \geq 0.$$

The proof is completed. □

Corollary 2.1. [16] *Let the DOC kernels $d^{(n)}_{n-k}$ be defined in* (10)*, it holds that*

$$\sum_{j=1}^{n} d^{(n)}_{n-j} \equiv \tau_n \quad \text{such that} \quad \sum_{k=1}^{n} \sum_{j=1}^{k} d^{(k)}_{k-j} \equiv t_n, \quad n \geq 1.$$

Lemma 2.6. *The DOC kernels* $d_{n-k}^{(n)}$ *defined in* (10) *have the following explicit formula*

$$d_{n-k}^{(n)} = \frac{1}{b_0^{(k)}} \prod_{i=k+1}^{n} \frac{(2\theta-1)\, r_i^2}{1+2\theta r_i} \geq 0, \quad 1 \leq k \leq n.$$

Proof. According to (10), it yields

$$\begin{aligned} -b_1^{(k+1)} d_{n-k-1}^{(n)} &= -\frac{b_1^{(k+1)}}{b_0^{(k+1)}} b_0^{(k+1)} d_{n-k-1}^{(n)} \\ &= -\frac{b_1^{(k+1)}}{b_0^{(k+1)}} \left(-b_1^{(k+2)} d_{n-k-2}^{(n)}\right) = \prod_{i=k+1}^{n} \left(-\frac{b_1^{(i)}}{b_0^{(i)}}\right). \end{aligned}$$

From (10) and (9), we obtain

$$d_{n-k}^{(n)} = -\frac{b_1^{(k+1)}}{b_0^{(k)}} d_{n-k-1}^{(n)} = \frac{1}{b_0^{(k)}} \prod_{i=k+1}^{n} \left(-\frac{b_1^{(i)}}{b_0^{(i)}}\right) = \frac{1}{b_0^{(k)}} \prod_{i=k+1}^{n} \frac{(2\theta-1) r_i^2}{1+2\theta r_i}, \ 1 \leq k \leq n.$$

The proof is completed. □

3. The unique solvability and energy stability

Let $H^m(\Omega)$ and $\|\cdot\|_{H^m(\Omega)}$ denote the standard Sobolev spaces and their associated norms, respectively. In particular, $(\cdot,\cdot)$ and $\|\cdot\|$ represent the usual inner product and norm in the space $L^2(\Omega)$, respectively.

3.1. The unique solvability.

First, we establish the unique solvability of the WSBDF2 method (6) via a discrete energy functional for the Allen-Cahn equation (1).

Theorem 3.1. *If the time-step size satisfies* $\tau_n < \frac{1+2\theta r_n}{\theta(1+r_n)}$ *for* $n \geq 1$*, then the WSBDF2 method* (6) *is uniquely solvable.*

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

$$\begin{aligned} G[z] := &\frac{b_0^{(n)}}{2} \left\|z - u^{n-1}\right\|^2 + \left(b_1^{(n)} \nabla_\tau u^{n-1}, z - u^{n-1}\right) + \frac{\theta\varepsilon^2}{2} \|\nabla z\|^2 \\ &- (1-\theta)\,\varepsilon^2 \left(\Delta u^{n-1}, z\right) + \frac{\theta}{8} \|z\|_{L^4}^4 + \frac{\theta}{4} \left(\left(u^{n-1}\right)^2, z^2\right) + \frac{\theta}{6} \left(u^{n-1}, z^3\right) \\ &+ \left(1 - \frac{3\theta}{2}\right) \left(\left(u^{n-1}\right)^3, z\right) - \frac{\theta}{2} \|z\|^2 + (\theta - 1) \left(u^{n-1}, z\right). \end{aligned}$$

If the time-step size satisfies $\tau_n < \frac{1+2\theta r_n}{\theta(1+r_n)}$, we obtain $b_0^{(n)} > \theta$ by definition (9). Then, the functional G is strictly convex. In fact, for any $\lambda \in \mathbb{R}$ and ψ, one has

$$\begin{aligned} \frac{d^2 G}{d\lambda^2}[z + \lambda\psi]\Big|_{\lambda=0} &= b_0^{(n)} \|\psi\|^2 + \theta\varepsilon^2 \|\nabla\psi\|^2 + \theta \|z\psi\|^2 - \theta \|\psi\|^2 \\ &+ \frac{\theta}{2} \left\|\left(z + u^{n-1}\right)\psi\right\|^2 \geq \left(b_0^{(n)} - \theta\right) \|\psi\|^2 > 0. \end{aligned}$$

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

$$\begin{aligned} 0 = & \frac{dG}{d\lambda}[z+\lambda\psi]\Big|_{\lambda=0} \\ = & \left(b_0^{(n)}\left(z-u^{n-1}\right)+b_1^{(n)}\nabla_\tau u^{n-1}-\theta\varepsilon^2\Delta z-(1-\theta)\,\varepsilon^2\Delta u^{n-1},\psi\right) \\ & +\frac{\theta}{2}\left(z^3+\left(u^{n-1}\right)^2 z+u^{n-1}z^2-\left(u^{n-1}\right)^3,\psi\right)-\theta\,(z,\psi) \\ & +(1-\theta)\left(\left(u^{n-1}\right)^3-u^{n-1},z\right). \end{aligned}$$

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

$$b_0^{(n)}\left(u^n-u^{n-1}\right)+b_1^{(n)}\nabla_\tau u^{n-1}-\varepsilon^2\left(\theta\Delta u^n+(1-\theta)\,\Delta u^{n-1}\right)+H(u^n)=0,$$

which is the WSBDF2 method (6). □

3.2. The discrete energy dissipation law. Let $E(u^k)$ be the discrete version of free energy functional (2), which is defined by

$$E(u^k)=\frac{\varepsilon^2}{2}\left\|\nabla u^k\right\|^2+\frac{1}{4}\left\|(u^k)^2-1\right\|^2,\quad 0\le k\le N. \tag{20}$$

Denote the modified discrete energy $\mathcal{E}(u^k)$ by

$$\mathcal{E}(u^k)=\frac{(2\theta-1)\,r_{k+1}^{3/2}}{2\,(1+r_{k+1})}\frac{\left\|\nabla_\tau u^k\right\|^2}{\tau_k}+E(u^k),\quad k\ge 1 \tag{21}$$

with the initial energy $\mathcal{E}(u^0):=E(u^0)$, which corresponds to the setting $r_1=0$.

The following theorem demonstrates that the WSBDF2 scheme (6) preserves a modified energy dissipation law at the discrete levels, which implies the energy stability.

Theorem 3.2. *Let the adjacent time-step ratios r_n satisfy $0<r_n\le r_s$ in (17) for $2\le n\le N$. If the time-step sizes are properly small such that*

$$\tau_n\le\min\left\{\frac{1+2\theta r_n}{\theta(1+r_n)},\frac{h(r_n,r_{n+1})}{2\theta-1}\right\},\quad n\ge 1. \tag{22}$$

Then the WSBDF2 scheme (6) preserves the following energy dissipation law

$$\mathcal{E}(u^n)\le\mathcal{E}(u^{n-1}),\quad n\ge 1. \tag{23}$$

Proof. The first condition of (22) ensures the unique solvability. We will establish the energy dissipation law under the second condition of (22). Making the inner product of (6) by $\nabla_\tau u^k$, we obtain

$$\left(\mathcal{D}_2 u^k,\nabla_\tau u^k\right)-\varepsilon^2\left(\theta\Delta u^k+\left(1-\theta\right)\Delta u^{k-1},\nabla_\tau u^k\right)+\left(H(u^k),\nabla_\tau u^k\right)=0. \tag{24}$$

According to (8) and Lemma 2.4, it yields

$$\begin{aligned} \left(\mathcal{D}_2 u^k,\nabla_\tau u^k\right)\ge & \frac{(2\theta-1)r_{k+1}^{3/2}}{2\left(1+r_{k+1}\right)}\frac{\left\|\nabla_\tau u^k\right\|^2}{\tau_k}-\frac{(2\theta-1)r_k^{3/2}}{2\left(1+r_k\right)}\frac{\left\|\nabla_\tau u^{k-1}\right\|^2}{\tau_{k-1}} \\ & +\frac{h\left(r_k,r_{k+1}\right)}{2}\frac{\left\|\nabla_\tau u^k\right\|^2}{\tau_k},\quad k\ge 2. \end{aligned}$$

With the help of the inequality $2a(a-b) \geq a^2 - b^2$, we have

$$\begin{aligned}
&-\varepsilon^2\big(\theta\Delta u^k + (1-\theta)\Delta u^{k-1}, \nabla_\tau u^k\big)\\
&= \varepsilon^2(1-\theta)\big(\nabla u^k + \nabla u^{k-1}, \nabla u^k - \nabla u^{k-1}\big) + \varepsilon^2(2\theta-1)\big(\nabla u^k, \nabla u^k - \nabla u^{k-1}\big)\\
&\geq \varepsilon^2(1-\theta)\big(\|\nabla u^k\|^2 - \|\nabla u^{k-1}\|^2\big) + \frac{\varepsilon^2(2\theta-1)}{2}\big(\|\nabla u^k\|^2 - \|\nabla u^{k-1}\|^2\big)\\
&= \frac{\varepsilon^2}{2}\|\nabla u^k\|^2 - \frac{\varepsilon^2}{2}\|\nabla u^{k-1}\|^2, \quad k \geq 1.
\end{aligned}$$

Let $f(a) = a^3 - a$, $F(a) = \frac{1}{4}(a^2-1)^2$. We can verify that

$$\begin{aligned}
f(a)(a-b) &= \frac{1}{4}\big[(a^2-1)^2 - (b^2-1)^2 - 2(1-a^2)(a-b)^2 + (a^2-b^2)^2\big],\\
f(b)(a-b) &= \frac{1}{4}\big[(a^2-1)^2 - (b^2-1)^2 + 2(1-b^2)(a-b)^2 - (a^2-b^2)^2\big].
\end{aligned}$$

Thus, it leads to

$$\begin{aligned}
&[\theta f(a) + (1-\theta)f(b)](a-b)\\
&= \frac{1}{4}(a^2-1)^2 - \frac{1}{4}(b^2-1)^2 + \frac{(a-b)^2}{2}[\theta(a^2-1) + (1-\theta)(1-b^2)]\\
&\quad + \frac{2\theta-1}{4}(a^2-b^2)^2\\
&\geq F(a) - F(b) + \frac{(a-b)^2}{2}[\theta(a^2-1) + (1-\theta)(1-b^2)], \quad \theta \in [1/2, 1].
\end{aligned}$$

According to (7) and the above inequality, it yields

$$\begin{aligned}
H(a)(a-b) &= [\theta f(a) + (1-\theta)f(b) - \frac{\theta}{2}(a+b)(a-b)^2](a-b)\\
&\geq F(a) - F(b) + \frac{(a-b)^2}{2}[\theta(a^2-1) + (1-\theta)(1-b^2)]\\
&\quad - \frac{\theta}{2}\left(a^2-b^2\right)(a-b)^2\\
&= F(a) - F(b) + \frac{(a-b)^2}{2}[1 - 2\theta + b^2(2\theta-1)]\\
&\geq F(a) - F(b) - \frac{2\theta-1}{2}(a-b)^2, \quad \theta \in [1/2, 1].
\end{aligned}$$

Therefore, taking $a = u^k$ and $b = u^{k-1}$ in the above inequality, we obtain

$$\big(H(u^k), \nabla_\tau u^k\big) \geq \frac{1}{4}\|(u^k)^2 - 1\|^2 - \frac{1}{4}\|(u^{k-1})^2 - 1\|^2 - \frac{2\theta-1}{2}\|\nabla_\tau u^k\|^2.$$

According to (24) and the above inequalities, one gets

$$\mathcal{E}(u^k) - \mathcal{E}(u^{k-1}) + \left(\frac{h(r_k, r_{k+1})}{2\tau_k} - \frac{2\theta-1}{2}\right)\|\nabla_\tau u^k\|^2 \leq 0, \quad k \geq 2.$$

Under the second condition of (22) yields

$$\mathcal{E}(u^k) \leq \mathcal{E}(u^{k-1}), \quad k \geq 2.$$

For the case $k = 1$, from (5), (24) and the above inequalities, we have

$$\frac{1}{\tau_1}\|\nabla_\tau u^1\|^2 + E(u^1) - E(u^0) - \frac{2\theta-1}{2}\|\nabla_\tau u^1\|^2 \leq 0.$$

Then the above inequality gives

$$\left(\frac{1}{\tau_1}-\frac{h(r_1,r_2)}{2\tau_1}\right)\left\|\nabla_\tau u^1\right\|^2+E(u^1)+\left(\frac{h(r_1,r_2)}{2\tau_1}-\frac{2\theta-1}{2}\right)\left\|\nabla_\tau u^1\right\|^2\le E(u^0).$$

Based on (19), we obtain

$$h(r_1,r_2)=h(0,r_2)=2-\frac{(2\theta-1)r_2^{3/2}}{1+r_2}.$$

Thus, it follows that

$$\frac{(2\theta-1)r_2^{3/2}}{1+r_2}\frac{\left\|\nabla_\tau u^1\right\|^2}{2\tau_1}+E(u^1)+\left(\frac{h(r_1,r_2)}{2\tau_1}-\frac{2\theta-1}{2}\right)\left\|\nabla_\tau u^1\right\|^2\le E(u^0).$$

From (21), one has

$$\mathcal{E}(u^1)+\left(\frac{h(r_1,r_2)}{2\tau_1}-\frac{2\theta-1}{2}\right)\left\|\nabla_\tau u^1\right\|^2\le E(u^0)=\mathcal{E}(u^0).$$

Under the second condition of (22) yields

$$\mathcal{E}(u^1)\le\mathcal{E}(u^0).$$

The desired result (23) is obtained. □

Remark 3.1. From the perspective of the energy technique [4], the Nevanlinna-Odeh multiplier is selected as $\mu_1=1$, namely, $\nabla_\tau u^k:=u^k-\mu_1 u^{k-1}$ in Theorem 3.2. Moreover, it should be noted that Lemma 2.4 is similar to G-stability for the two-step multistep method on variable grids.

Lemma 3.1. *Let the adjacent time-step ratios r_n satisfy $0<r_n\le r_s$ in* (17) *for $2\le n\le N$. If the step sizes τ_n satisfy* (22)*, the solution of the WSBDF2 method* (6) *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 the constant c_1 is dependent on the domain Ω, the interface parameter ε and the initial 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 (23), the definition (20) and (21), it yields

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

Thus, it follows that

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

The proof is completed. □

4. Stability analysis for WSBDF2 method

In this section, we establish the unconditional stability for the WSBDF2 method (6). First, we recall the discrete Gronwall's inequality, which is required in the subsequent analysis.

Lemma 4.1. [16] *Let $\lambda \geq 0$ and the sequences $\{\xi_k\}_{k=0}^N$ and $\{V_k\}_{k=1}^N$ be nonnegative. If*

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

then it holds that

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

Theorem 4.1. *Let u^n be the solution of the WSBDF2 method* (6)*, and ρ^n be the solution perturbation $\rho^n = \widetilde{u}^n - u^n$ for $0 \leq n \leq N$. Let the adjacent time-step ratios r_n satisfy $0 < r_n \leq r_s$ in* (17) *for $2 \leq n \leq N$ and the time-step sizes τ_n fulfill* (22) *such that the WSBDF2 scheme* (6) *is unique solvable and energy stable. If the time-step sizes $\tau_n \leq \frac{1}{4\theta(c_\phi + c_\varphi)}$, then the discrete solution u^n is unconditionally stable in the L^2 norm*

$$\|\rho^n\| \leq 3\exp\left(4\left(c_\phi + c_\varphi\right)T\right)\left\|\rho^0\right\|, \quad n \geq 1,$$

where the constant c_ϕ and c_φ are defined in (26) *and* (27)*, respectively, which are independent of the time t_n, the time-step sizes τ_n and the time-step ratios r_n.*

Proof. Based on the WSBDF2 method (6), we obtain the perturbed equation

(25)
$$\mathcal{D}_2\rho^j - \varepsilon^2\left(\theta\Delta\rho^j + (1-\theta)\Delta\rho^{j-1}\right) = H(u^j) - H(\widetilde{u}^j) = \phi^j\rho^j + \varphi^j\rho^{j-1}, \quad j \geq 1$$

with

$$\begin{aligned}
\phi^j &= -\frac{\theta}{2}\left(\left(u^j\right)^2 + u^j\widetilde{u}^j + \left(\widetilde{u}^j\right)^2 + \widetilde{u}^{j-1}u^j + \widetilde{u}^{j-1}\widetilde{u}^j + \left(u^{j-1}\right)^2 - 2\right),\\
\varphi^j &= -\frac{\theta}{2}\left(\left(u^j\right)^2 + \widetilde{u}^j u^{j-1} + \widetilde{u}^j\widetilde{u}^{j-1} - \left(u^{j-1}\right)^2 - u^{j-1}\widetilde{u}^{j-1} - \left(\widetilde{u}^{j-1}\right)^2\right)\\
&\quad + (\theta-1)\left(\left(u^{j-1}\right)^2 + u^{j-1}\widetilde{u}^{j-1} + \left(\widetilde{u}^{j-1}\right)^2 - 1\right).
\end{aligned}$$

Note that the solution estimates in Lemma 3.1 and $H^1 \subseteq L^\infty$, we have

(26)
$$\begin{aligned}
\left\|\phi^j\right\|_{L^\infty} &\leq \frac{\theta}{2}\big(\left\|u^j\right\|_{L^\infty}^2 + \left\|u^j\right\|_{L^\infty}\left\|\widetilde{u}^j\right\|_{L^\infty} + \left\|\widetilde{u}^j\right\|_{L^\infty}^2 + \left\|\widetilde{u}^{j-1}\right\|_{L^\infty}\left\|u^j\right\|_{L^\infty}\\
&\quad + \left\|\widetilde{u}^{j-1}\right\|_{L^\infty}\left\|\widetilde{u}^j\right\|_{L^\infty} + \left\|u^{j-1}\right\|_{L^\infty}^2 + 2\big)\\
&\leq \frac{\theta}{2}c_\Omega^2\big(\left\|u^j\right\|_{H^1}^2 + \left\|u^j\right\|_{H^1}\left\|\widetilde{u}^j\right\|_{H^1} + \left\|\widetilde{u}^j\right\|_{H^1}^2 + \left\|\widetilde{u}^{j-1}\right\|_{H^1}\left\|u^j\right\|_{H^1}\\
&\quad + \left\|\widetilde{u}^{j-1}\right\|_{H^1}\left\|\widetilde{u}^j\right\|_{H^1} + \left\|u^{j-1}\right\|_{H^1}^2\big) + \theta\\
&\leq \theta c_\Omega^2\big(c_1^2 + c_1\widetilde{c_1} + \widetilde{c_1}^2\big) + \theta := c_\phi, \quad j \geq 1,
\end{aligned}$$

where $\left\|\widetilde{u}^j\right\|_{H^1} \leq \widetilde{c_1}$ is similar to Lemma 3.1 and the constant c_Ω is dependent on the domain Ω, but independent of the time t_n, the time-step sizes τ_n and the time-step ratios r_n.

Following a similar approach as in (26), it yields

$$\left\|\varphi^j\right\|_{L^\infty} \leq c_\Omega^2\left(c_1^2 + c_1\widetilde{c_1} + \widetilde{c_1}^2\right) + (1-\theta) := c_\varphi, \quad j \geq 1. \tag{27}$$

Multiplying both sides of (25) by the DOC kernels $d_{k-j}^{(k)}$, and summing j from 1 to k, we derive

$$\sum_{j=1}^{k} d_{k-j}^{(k)} \mathcal{D}_2\rho^j - \varepsilon^2 \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\theta\Delta\rho^j + (1-\theta)\Delta\rho^{j-1}\right) = \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\phi^j\rho^j + \varphi^j\rho^{j-1}\right).$$

From (8) and the orthogonal identity (11), we get

$$\sum_{j=1}^{k} d_{k-j}^{(k)} \mathcal{D}_2\rho^j = \sum_{j=1}^{k} d_{k-j}^{(k)} \sum_{l=1}^{j} b_{j-l}^{(j)} \nabla_\tau\rho^l = \sum_{l=1}^{k} \nabla_\tau\rho^l \sum_{j=l}^{k} d_{k-j}^{(k)} b_{j-l}^{(j)} = \nabla_\tau\rho^k, \quad k \geq 1.$$

Thus, it follows that

$$\nabla_\tau\rho^k - \varepsilon^2 \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\theta\Delta\rho^j + (1-\theta)\Delta\rho^{j-1}\right) = \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\phi^j\rho^j + \varphi^j\rho^{j-1}\right).$$

Taking the inner product of the above equality with $v^k = \theta\rho^k + (1-\theta)\rho^{k-1}$ and summing the resulting equality from $k=1$ to n, we obtain

$$\begin{aligned} &\sum_{k=1}^{n} \left(\nabla_\tau\rho^k, v^k\right) - \varepsilon^2 \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \left(\theta\Delta\rho^j + (1-\theta)\Delta\rho^{j-1}, v^k\right) \\ &= \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \left(\phi^j\rho^j + \varphi^j\rho^{j-1}, v^k\right). \end{aligned}$$

For the first term on the left hand, we get

$$\begin{aligned} \sum_{k=1}^{n} \left(\nabla_\tau\rho^k, v^k\right) &= \sum_{k=1}^{n} \left(\rho^k - \rho^{k-1}, \theta\rho^k + (1-\theta)\rho^{k-1}\right) \\ &= \sum_{k=1}^{n} \left[(1-\theta)\left(\rho^k - \rho^{k-1}, \rho^k + \rho^{k-1}\right) + (2\theta-1)\left(\rho^k - \rho^{k-1}, \rho^k\right)\right] \\ &\geq \frac{1}{2}\sum_{k=1}^{n} \left(\left\|\rho^k\right\|^2 - \left\|\rho^{k-1}\right\|^2\right) = \frac{1}{2}\left\|\rho^n\right\|^2 - \frac{1}{2}\left\|\rho^0\right\|^2, \end{aligned}$$

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

For the second term on the left hand, we obtain

$$\begin{aligned} &-\varepsilon^2 \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \left(\theta\Delta\rho^j + (1-\theta)\Delta\rho^{j-1}, v^k\right) \\ &= \varepsilon^2 \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \left(\theta\nabla\rho^j + (1-\theta)\nabla\rho^{j-1}, \theta\nabla\rho^k + (1-\theta)\nabla\rho^{k-1}\right) \geq 0, \end{aligned}$$

where the Lemma 2.5 has been used.

It is noted that Lemma 2.6 shows $d_{k-j}^{(k)} \geq 0$. Combining the above estimates and the Cauchy-Schwarz inequality, it follows that

$$\begin{aligned}\|\rho^n\|^2 &\leq \|\rho^0\|^2 + 2\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \|\phi^j\rho^j + \varphi^j\rho^{j-1}\| \|\theta\rho^k + (1-\theta)\rho^{k-1}\| \\ &\leq \|\rho^0\|^2 + 2\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \big(c_\phi\|\rho^j\| + c_\varphi\|\rho^{j-1}\|\big)\big(\theta\|\rho^k\| + (1-\theta)\|\rho^{k-1}\|\big).\end{aligned}$$

Taking some integer n_1 $(0 \leq n_1 \leq n)$ such that $\|\rho^{n_1}\| = \max_{0\leq k\leq n} \|\rho^k\|$. Setting $n := n_1$ in the above inequality yields

$$\|\rho^{n_1}\|^2 \leq \|\rho^0\|\|\rho^{n_1}\| + 2\big(c_\phi + c_\varphi\big)\|\rho^{n_1}\| \sum_{k=1}^{n_1}\sum_{j=1}^{k} d_{k-j}^{(k)} \big(\theta\|\rho^k\| + (1-\theta)\|\rho^{k-1}\|\big).$$

Using Corollary 2.1, we have

$$\begin{aligned}\|\rho^n\| &\leq \|\rho^0\| + 2\big(c_\phi + c_\varphi\big)\sum_{k=1}^{n} \tau_k \big(\theta\|\rho^k\| + (1-\theta)\|\rho^{k-1}\|\big) \\ &= \big(1 + 2\big(c_\phi + c_\varphi\big)(1-\theta)\tau_1\big)\|\rho^0\| + 2\big(c_\phi + c_\varphi\big)\theta\tau_n\|\rho^n\| \\ &\quad + 2\big(c_\phi + c_\varphi\big)\sum_{k=1}^{n-1}\big(\theta\tau_k + (1-\theta)\tau_{k+1}\big)\|\rho^k\|.\end{aligned}$$

Using the discrete Gronwall's inequality in Lemma 4.1 and for sufficiently small step-sizes τ_n, i.e., $2\big(c_\phi + c_\varphi\big)\theta\tau_n < \frac{1}{2}$, we get

$$\|\rho^n\| \leq 2\big(1 + 2\big(c_\phi + c_\varphi\big)(1-\theta)\tau_1\big)\exp\big(4\big(c_\phi + c_\varphi\big)T\big)\|\rho^0\|, \quad n \geq 1.$$

The proof is completed. □

5. Convergence analysis for WSBDF2 method

In this section, we are ready to present the L^2 norm convergence analysis. To begin with, we consider the local consistency error of the WSBDF2 method (6).

Lemma 5.1. *Let the consistency error be defined by*

$$\eta^j := \mathcal{D}_2 u(t_j) - \theta\partial_t u(t_j) - (1-\theta)\partial_t u(t_{j-1}).$$

Then, it holds that

$$\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}\|\eta^j\| \leq 2(2-\theta)\tau_{\max}\int_0^{t_1}\|\partial_{tt}u\|\,dt + 3t_n \max_{1\leq j\leq n}\tau_j\int_{t_{j-1}}^{t_j}\|\partial_{ttt}u\|\,dt,\ n \geq 1$$

with $\tau_{\max} = \max_{1\leq k\leq N}\tau_k$.

Proof. For simplicity, we denote

$$G_{t2}^j = \int_{t_{j-1}}^{t_j}\|\partial_{tt}u\|\,dt, \quad G_{t3}^j = \int_{t_{j-1}}^{t_j}\|\partial_{ttt}u\|\,dt,\ j \geq 1.$$

For $j = 1$, based on (5) and Taylor's expansion formula, we obtain

$$\begin{aligned}\eta^1 =& \frac{u(t_1) - u(t_0)}{\tau_1} - \theta\partial_t u(t_1) - (1-\theta)\partial_t u(t_0) \\ =& (1-\theta)\int_0^{t_1}\partial_{tt}u\,dt - \frac{1}{\tau_1}\int_0^{t_1} t\partial_{tt}u\,dt.\end{aligned}$$

Then the consistency error is bounded by

$$\left\|\eta^1\right\| \le (1-\theta)\, G_{t2}^1 + G_{t2}^1 = (2-\theta)\, G_{t2}^1.$$

For $j \ge 2$, according to (8) and Taylor's expansion formula, we get

$$\begin{aligned}
\eta^j &= b_0^{(j)}\left(u(t_j)-u(t_{j-1})\right) + b_1^{(j)}\left(u(t_{j-1})-u(t_{j-2})\right) - \theta\partial_t u\left(t_j\right) - (1-\theta)\,\partial_t u\left(t_{j-1}\right)\\
&= \frac{(1+2\theta r_j) - (1-2\theta)\, r_j^2}{2\tau_j\,(1+r_j)} \int_{t_{j-1}}^{t_j} \left(t-t_{j-1}\right)^2 \partial_{ttt} u dt\\
&\quad + \frac{(1-2\theta)\, r_j^2}{2\tau_j\,(1+r_j)} \int_{t_{j-2}}^{t_j} \left(t-t_{j-2}\right)^2 \partial_{ttt} u dt + (1-\theta)\int_{t_{j-1}}^{t_j} \left(t_{j-1}-t\right) \partial_{ttt} u dt\\
&= \frac{1}{2}\left(b_0^{(j)} - b_1^{(j)}\right) \int_{t_{j-1}}^{t_j} \left(t-t_{j-1}\right)^2 \partial_{ttt} u dt + \frac{1}{2} b_1^{(j)} \int_{t_{j-2}}^{t_{j-1}} \left(t-t_{j-2}\right)^2 \partial_{ttt} u dt\\
&\quad + \frac{1}{2} b_1^{(j)} \int_{t_{j-1}}^{t_j} \left(t-t_{j-1}+\tau_{j-1}\right)^2 \partial_{ttt} u dt + (1-\theta)\int_{t_{j-1}}^{t_j} \left(t_{j-1}-t\right) \partial_{ttt} u dt\\
&= \frac{1}{2} b_0^{(j)} \int_{t_{j-1}}^{t_j} \left(t-t_{j-1}\right)^2 \partial_{ttt} u dt + \frac{1}{2} b_1^{(j)} \int_{t_{j-2}}^{t_{j-1}} \left(t-t_{j-2}\right)^2 \partial_{ttt} u dt\\
&\quad + \frac{1}{2} b_1^{(j)} \tau_{j-1} \int_{t_{j-1}}^{t_j} \left(2\left(t-t_{j-1}\right)+\tau_{j-1}\right) \partial_{ttt} u dt + (1-\theta)\int_{t_{j-1}}^{t_j} \left(t_{j-1}-t\right) \partial_{ttt} u dt.
\end{aligned}$$

Then the consistency error is bounded by

$$\begin{aligned}
\left\|\eta^j\right\| &\le \frac{1}{2} b_0^{(j)} \tau_j^2 G_{t3}^j - \frac{1}{2} b_1^{(j)} \tau_{j-1}^2 G_{t3}^{j-1} - \frac{1}{2} b_1^{(j)} \tau_{j-1}\left(2\tau_j + \tau_{j-1}\right) G_{t3}^j + (1-\theta)\,\tau_j G_{t3}^j\\
&= \frac{1}{2} b_0^{(j)} \tau_j^2 G_{t3}^j \left(1 - \frac{b_1^{(j)}\left(1+2r_j\right)}{b_0^{(j)} r_j^2} + \frac{2\,(1-\theta)}{b_0^{(j)}\tau_j}\right) - \frac{b_1^{(j)}\tau_{j-1}^2}{2 b_0^{(j)}} b_0^{(j)} G_{t3}^{j-1}\\
&= b_0^{(j)} \tau_j^2 G_{t3}^j + \frac{(2\theta-1)\, r_j^2 \tau_{j-1}^2}{2\left(1+2\theta r_j\right)} b_0^{(j)} G_{t3}^{j-1}, \quad j \ge 2.
\end{aligned}$$

From (10) and (9), it leads to

$$d_{k-j}^{(k)} b_0^{(j)} = -d_{k-j-1}^{(k)} b_1^{(j+1)} = \frac{(2\theta-1)\, r_{j+1}^2}{1+2\theta r_{j+1}} d_{k-j-1}^{(k)} b_0^{(j+1)}, \quad 1 \le j \le k-1.$$

Combining the above estimates, one has

$$\begin{aligned}
&\sum_{j=1}^{k} d_{k-j}^{(k)} \left\|\eta^j\right\| = d_{k-1}^{(k)} \left\|\eta^1\right\| + \sum_{j=2}^{k} d_{k-j}^{(k)} \left\|\eta^j\right\|\\
&\le d_{k-1}^{(k)}\,(2-\theta)\, G_{t2}^1 + \sum_{j=2}^{k} d_{k-j}^{(k)} b_0^{(j)} \tau_j^2 G_{t3}^j + \frac{1}{2}\sum_{j=1}^{k-1} d_{k-j-1}^{(k)} b_0^{(j+1)} \frac{(2\theta-1)\, r_{j+1}^2}{1+2\theta r_{j+1}} \tau_j^2 G_{t3}^j\\
&= d_{k-1}^{(k)}\,(2-\theta)\, G_{t2}^1 + \sum_{j=2}^{k} d_{k-j}^{(k)} b_0^{(j)} \tau_j^2 G_{t3}^j + \frac{1}{2}\sum_{j=1}^{k-1} d_{k-j}^{(k)} b_0^{(j)} \tau_j^2 G_{t3}^j\\
&\le d_{k-1}^{(k)}\,(2-\theta)\, G_{t2}^1 + \frac{3}{2}\sum_{j=1}^{k} d_{k-j}^{(k)} b_0^{(j)} \tau_j^2 G_{t3}^j, \quad k \ge 1.
\end{aligned}$$

Applying Lemma 2.6 gives

$$d_{k-1}^{(k)} = \frac{1}{b_0^{(1)}} \prod_{i=2}^{k} \frac{(2\theta-1)r_i^2}{1+2\theta r_i} \leq \tau_1 \prod_{i=2}^{k} \frac{r_i^2}{1+2r_i} = \tau_k \prod_{i=2}^{k} \frac{r_i}{1+2r_i} \leq \frac{\tau_k}{2^{k-1}}.$$

Thus, it follows that

$$\sum_{k=1}^{n} d_{k-1}^{(k)} \leq \sum_{k=1}^{n} \frac{\tau_k}{2^{k-1}} \leq \tau_{\max} \sum_{k=1}^{n} \frac{1}{2^{k-1}} \leq 2\tau_{\max}, \quad \tau_{\max} = \max_{1\leq k\leq N} \tau_k.$$

From the above inequalities and Corollary 2.1, we derive

$$\begin{aligned}\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \left\|\eta^j\right\| &\leq \sum_{k=1}^{n} d_{k-1}^{(k)} (2-\theta)\, G_{t2}^1 + 3\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \tau_j G_{t3}^j \\ &\leq 2\,(2-\theta)\,\tau_{\max} \int_0^{t_1} \|\partial_{tt} u\|\, dt + 3t_n \max_{1\leq j\leq n} \tau_j \int_{t_{j-1}}^{t_j} \|\partial_{ttt} u\|\, dt.\end{aligned}$$

The proof is completed. □

Let $R^j = H(u(t_j)) - \theta f(u(t_j)) - (1-\theta) f(u(t_{j-1}))$ be the consistency error of the nonlinear term. According to (7), we have

$$R^j = -\frac{\theta}{2}\left(u(t_j) + u(t_{j-1})\right)\left(u(t_j) - u(t_{j-1})\right)^2.$$

The energy dissipation law (3) of the Allen-Cahn equation shows that $E(u(t_n)) \leq E(u(t_0))$. From the formulation (2), it is easy to check that $\|u(t_n)\|_{H^1}$ can be bounded by a time-independent constant c_2. Using $H^1 \subseteq L^\infty$ yields

$$\begin{aligned}\left\|R^j\right\| &\leq \frac{\theta}{2}\left(\left\|u(t_j)\right\|_{L^\infty} + \left\|u(t_{j-1})\right\|_{L^\infty}\right)\left\|\left(u(t_j)-u(t_{j-1})\right)^2\right\| \\ &\leq \frac{\theta}{2} c_\Omega \left(\left\|u(t_j)\right\|_{H^1} + \left\|u(t_{j-1})\right\|_{H^1}\right)\left\|\left(u(t_j)-u(t_{j-1})\right)^2\right\| \\ &\leq \theta c_2 c_\Omega \left\|\left(\int_{t_{j-1}}^{t_j} \partial_t u dt\right)^2\right\| \leq \theta c_2 c_\Omega \tau_j \left\|\int_{t_{j-1}}^{t_j} \left(\partial_t u\right)^2 dt\right\| \\ &\leq \theta c_2 c_\Omega \tau_j \int_{t_{j-1}}^{t_j} \left\|\left(\partial_t u\right)^2\right\| dt.\end{aligned}$$

Applying Corollary 2.1 gives

$$\begin{aligned}\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \left\|R^j\right\| &\leq \theta c_2 c_\Omega \sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)} \tau_j \int_{t_{j-1}}^{t_j} \left\|\left(\partial_t u\right)^2\right\| dt \\ &\leq \theta c_2 c_\Omega t_n \max_{1\leq j\leq n} \tau_j \int_{t_{j-1}}^{t_j} \left\|\left(\partial_t u\right)^2\right\| dt.\end{aligned} \tag{28}$$

Theorem 5.1. *Let $u(t_n)$ and u^n be the solution of the Allen-Cahn equation* (1) *and the WSBDF2 method* (6)*, respectively. Let the adjacent time-step ratios r_n satisfy $0 < r_n \leq r_s$ in* (17) *for $2 \leq n \leq N$ and the time-step sizes τ_n fulfill* (22) *such that the WSBDF2 scheme* (6) *is unique solvable and energy stable. If the time-step sizes $\tau_n \leq \frac{1}{4\theta(\widetilde{c}_\phi + \widetilde{c}_\varphi)}$, then the time-discrete solution u^n is convergent in the L^2 norm*

$$\left\|u(t_n) - u^n\right\| \leq C\tau_{\max} \int_0^{t_1} \left\|\partial_{tt} u\right\| dt + Ct_n \max_{1\leq j\leq n} \tau_j \int_{t_{j-1}}^{t_j} \left(\left\|\partial_{ttt} u\right\| + \left\|\left(\partial_t u\right)^2\right\|\right) dt,$$

where the constant $\widetilde{c}_\phi$ and $\widetilde{c}_\varphi$ are defined in (29) *and* (30)*, respectively, which are independent of the time t_n, the time-step sizes τ_n and the time-step ratios r_n.*

Proof. Let $e^n = u(t_n) - u^n$ be the error function with $e^0 = 0$. From (1) and (6), we obtain the error equation

$$\begin{aligned}\mathcal{D}_2 e^j - \varepsilon^2 \left(\theta \Delta e^j + (1-\theta)\, \Delta e^{j-1}\right) &= H(u^j) - H\left(u\left(t_j\right)\right) + \eta^j + R^j \\ &= \widetilde{\phi}^j e^j + \widetilde{\varphi}^j e^{j-1} + \eta^j + R^j, \quad j \geq 1\end{aligned}$$

with

$$\begin{aligned}\widetilde{\phi}^j &= -\frac{\theta}{2}\left[\left(u^j\right)^2 + u^j u(t_j) + (u(t_j))^2 + u(t_{j-1}) u^j + u(t_{j-1}) u(t_j) + \left(u^{j-1}\right)^2 - 2\right],\\ \widetilde{\varphi}^j &= -\frac{\theta}{2}\left[\left(u^j\right)^2 + u(t_j) u^{j-1} + u(t_j) u(t_{j-1}) - \left(u^{j-1}\right)^2 - u^{j-1} u(t_{j-1}) - \left(u(t_{j-1})\right)^2\right]\\ &\quad + (\theta - 1)\left[\left(u^{j-1}\right)^2 + u^{j-1} u(t_{j-1}) + \left(u(t_{j-1})\right)^2 - 1\right].\end{aligned}$$

Note that the solution estimates in Lemma 3.1 and $H^1 \subseteq L^\infty$, we have

(29)

$$\begin{aligned}\left\|\widetilde{\phi}^j\right\|_{L^\infty} &\leq \frac{\theta}{2}\Big(\left\|u^j\right\|_{L^\infty}^2 + \left\|u^j\right\|_{L^\infty}\left\|u(t_j)\right\|_{L^\infty} + \left\|u(t_j)\right\|_{L^\infty}^2 + \left\|u(t_{j-1})\right\|_{L^\infty}\left\|u^j\right\|_{L^\infty}\\ &\quad + \left\|u(t_{j-1})\right\|_{L^\infty}\left\|u(t_j)\right\|_{L^\infty} + \left\|u^{j-1}\right\|_{L^\infty}^2 + 2\Big)\\ &\leq \frac{\theta}{2} c_\Omega^2 \Big(\left\|u^j\right\|_{H^1}^2 + \left\|u^j\right\|_{H^1}\left\|u(t_j)\right\|_{H^1} + \left\|u(t_j)\right\|_{H^1}^2 + \left\|u(t_{j-1})\right\|_{H^1}\left\|u^j\right\|_{H^1}\\ &\quad + \left\|u(t_{j-1})\right\|_{H^1}\left\|u(t_j)\right\|_{H^1} + \left\|u^{j-1}\right\|_{H^1}^2\Big) + \theta\\ &\leq \theta c_\Omega^2 \left(c_1^2 + c_1 c_2 + c_2^2\right) + \theta := \widetilde{c}_\phi, \quad j \geq 1.\end{aligned}$$

Following the similar approach in (29), it leads to

$$\left\|\widetilde{\varphi}^j\right\|_{L^\infty} \leq c_\Omega^2 \left(c_1^2 + c_1 c_2 + c_2^2\right) + (1-\theta) := \widetilde{c}_\varphi, \quad j \geq 1. \tag{30}$$

By proceeding in a similar manner to that in Theorem 4.1, one has

$$\begin{aligned}\left\|e^n\right\|^2 &\leq 2 \sum_{k=1}^{n} \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\left\|\widetilde{\phi}^j e^j + \widetilde{\varphi}^j e^{j-1}\right\| + \left\|\eta^j + R^j\right\|\right)\left\|\theta e^k + (1-\theta) e^{k-1}\right\|\\ &\leq 2 \sum_{k=1}^{n} \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\widetilde{c}_\phi \left\|e^j\right\| + \widetilde{c}_\varphi \left\|e^{j-1}\right\| + \left\|\eta^j\right\| + \left\|R^j\right\|\right)\left\|\theta e^k + (1-\theta) e^{k-1}\right\|.\end{aligned}$$

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

$$\left\|e^{n_2}\right\|^2 \leq 2\left\|e^{n_2}\right\| \sum_{k=1}^{n_2} \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\left(\widetilde{c}_\phi + \widetilde{c}_\varphi\right)\left\|\theta e^k + (1-\theta) e^{k-1}\right\| + \left\|\eta^j\right\| + \left\|R^j\right\|\right).$$

According to Corollary 2.1 gives

$$\begin{aligned}\left\|e^n\right\| &\leq 2\left(\widetilde{c}_\phi + \widetilde{c}_\varphi\right) \sum_{k=1}^{n} \tau_k \left\|\theta e^k + (1-\theta) e^{k-1}\right\| + 2 \sum_{k=1}^{n} \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\left\|\eta^j\right\| + \left\|R^j\right\|\right)\\ &= 2\left(\widetilde{c}_\phi + \widetilde{c}_\varphi\right) \sum_{k=1}^{n-1} \left(\theta\tau_k + (1-\theta)\tau_{k+1}\right) \left\|e^k\right\| + 2 \sum_{k=1}^{n} \sum_{j=1}^{k} d_{k-j}^{(k)} \left(\left\|\eta^j\right\| + \left\|R^j\right\|\right)\\ &\quad + 2\left(\widetilde{c}_\phi + \widetilde{c}_\varphi\right)\theta\tau_n\left\|e^n\right\|.\end{aligned}$$

Applying the discrete Gronwall's inequality in Lemma 4.1 and provided that the step-sizes τ_n are sufficiently small, i.e., $2\,(\widetilde{c}_\phi + \widetilde{c}_\varphi)\,\theta\tau_n < \frac{1}{2}$, we have

$$\|e^n\| \le 4\exp\big(4(\widetilde{c}_\phi + \widetilde{c}_\varphi)T\big)\sum_{k=1}^{n}\sum_{j=1}^{k} d_{k-j}^{(k)}\big(\|\eta^j\| + \|R^j\|\big), \quad n \ge 1.$$

The desired result can be immediately derived from Lemma 5.1 and (28). □

6. Numerical experiments

In this section, we provide details on the numerical implementations and present several numerical examples to validate our theoretical results. For the WSBDF2 method (6), we carry out a simple Newton-type iteration at each time level with a tolerance 10^{-10}. We select the solution at the previous level as the initial value of Newton iteration. In space, we discretize by the spectral collocation method with the Chebyshev–Gauss–Lobatto points [4, 19]. We express the space discrete approximation u_I^n in terms of its values at Chebyshev–Gauss–Lobatto points,

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

where $u_{ij}^n := u_I^n(x_i, y_j)$ at the mesh points (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., [19, Theorem 4.4, §4.5.2].

The initial value and the forcing term are chosen such that the exact solution of equation (1) is

$$u(x,y,t) = (t^3+1)\cos(\pi x)\cos(\pi y), \quad -1 \leqslant x, y \leqslant 1, \quad 0 \leqslant t \leqslant 1$$

with the periodic boundary conditions

$$u(-1,y,t) = u(1,y,t) = -(t^3+1)\cos(\pi y),$$
$$u(x,-1,t) = u(x,1,t) = -(t^3+1)\cos(\pi x).$$

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

Case I: $r_{2k} = 4$, for $1 \le k \le \frac{N}{2}$, and $r_{2k-1} = 1/4$, for $2 \le k \le \frac{N}{2}$.

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 [16].

As is observed in Table 6, the WSBDF2 method (6) achieves second-order accuracy on nonuniform meshes, even for the cases with the adjacent time-step ratios $r_n > r_s$ in (17). The same phenomena have also been observed for the variable two- and three-step BDF method in [15, 9], respectively. The numerical experiments indicate that the WSBDF2 method is much more robust with respect to the step-size variations than previously predicted by theory. In addition, r_s in (17) may be not the optimal upper bound on the adjacent time-step ratios, and deserves further investigation. Noted that we shall adopt an adaptive time-stepping strategy by Algorithm 1 in [15] to choose the time-step size in the numerical experiments.

TABLE 1. Example 6.1: Errors and orders of convergence with $\varepsilon = 0.02$.

Case I								
N	$\theta = 1/2$	Rate	$\theta = 3/4$	Rate	$\theta = 1$	Rate	$\max r_k$	$\min r_k$
800	3.6798e-06		4.5492e-06		5.4262e-06		4	1/4
1600	9.1893e-07	2.00	1.1367e-06	2.00	1.3564e-06	2.00	4	1/4
3200	2.2960e-07	2.00	2.8409e-07	2.00	3.3909e-07	2.00	4	1/4
6400	5.7384e-08	2.00	7.1011e-08	2.00	8.4768e-08	2.00	4	1/4
Case II								
N	$\theta = 1/2$	Rate	$\theta = 3/4$	Rate	$\theta = 1$	Rate	$\max r_k$	$\min r_k$
800	3.5354e-06		5.3088e-06		6.9235e-06		504	6.19e-03
1600	8.8554e-07	1.99	1.3141e-06	2.01	1.7050e-06	2.02	3290	6.08e-05
3200	2.1642e-07	2.03	3.2009e-07	2.03	4.1555e-07	2.03	3290	6.08e-05
6400	5.5103e-08	1.97	8.1870e-08	1.96	1.0628e-07	1.96	3290	6.08e-05

Example 6.2. We focus on the Allen-Cahn model (1) with a diffusion coefficient of $\varepsilon = 0.02$. The WSBDF2 method (6) with $\theta = 0.8$ is utilized to simulate the merging of four bubbles with an initial condition [9]

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

and the periodic boundary conditions

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

The computational domain is $\Omega = (-1,1)^2$ with $M_x = M_y = 70$.

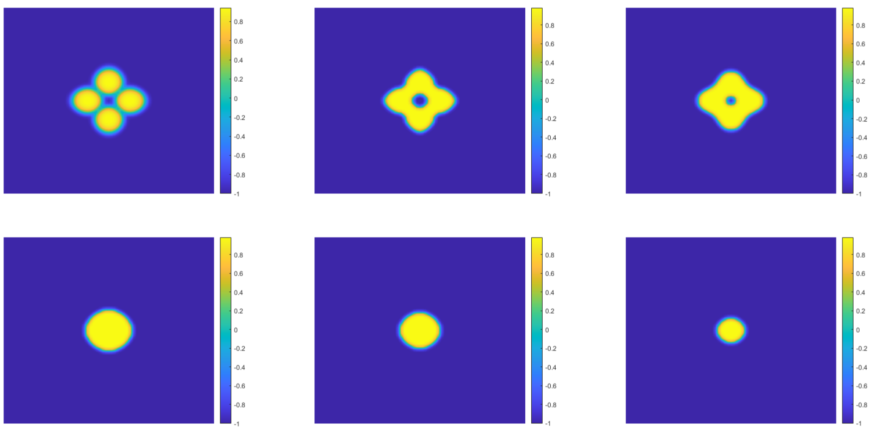

FIGURE 3. Solution snapshots of the Allen-Cahn equation using the arbitrary meshes at $t = 0, 10, 20, 140, 200, 290$ (from left to right), respectively.

We use the arbitrary meshes with random time-steps $\tau_k = T\sigma_k/S$ for $1 \le k \le N$. Here $S = \sum_{k=1}^{N} \sigma_k$, $T = 300$, $N = 30000$, $\theta = 4/5$ and $\sigma_k \in (0,1)$ are random numbers subject to the uniform distribution. The time evolution of the phase variable is shown in Figure 3. We observe that the initially separated four bubbles gradually merge into a single bubble. At the same time, the volume becomes smaller as time goes by due to the fact that the Allen-Cahn model does not preserve the volume conservation.

Example 6.3. We investigate the coarsening dynamics of the Allen-Cahn model (1) with the diffusion coefficient $\varepsilon = 0.02$ by employing arbitrary meshes with random time-step sizes until $T = 300$. The random initial condition is chosen as $u_0(x, y) = -0.5 + rand(x, y)$ for the WSBDF2 method (6) with $\theta = 0.8$ and $N = 30000$. The computational domain is $\Omega = (-1, 1)^2$ with $M_x = M_y = 70$, as stated in [9].

The time evolution of the coarsening dynamic is depicted in Figure 4. We notice that the microstructure is composed of a large number of grains at $t = 0$. As time progresses, the coarsening dynamics can be observed, including the migration of the phase boundaries, the process of decomposition, and the merging procedure. Moreover, it is noted that the number of grains gradually decreases over time.

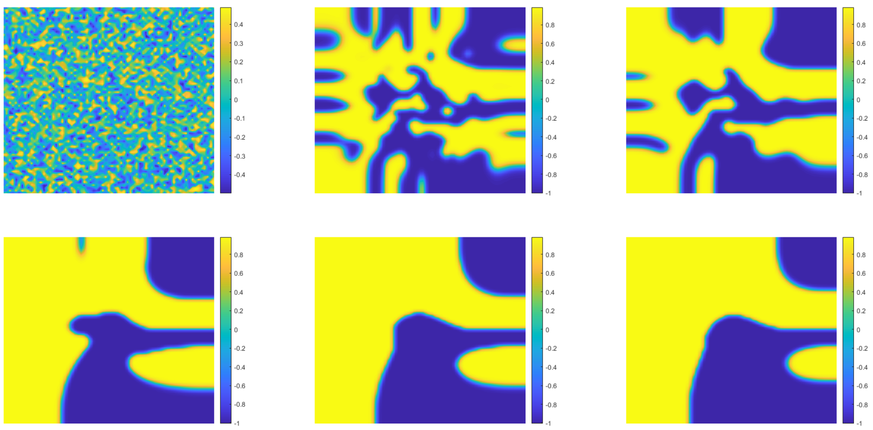

FIGURE 4. Solution snapshots of coarsening dynamic of the Allen-Cahn equation using the arbitrary meshes at $t = 0, 10, 20, 100, 200, 300$ (from left to right), respectively.

7. Conclusions

We have constructed the WSBDF2 method by the weighted and shifted technique, which is a flexible form between the Crank-Nicolson and two-step BDF methods. The energy stability of the proposed method is established on nonuniform meshes with the adjacent time-step ratios $r_n \leq r_s$ in (17). Moreover, the stability and convergence of the WSBDF2 method are rigorously proved, which fill in the gap of the theory for PDEs in [21]. The powerful weighted and shifted technique offers a flexible framework to construct high-order schemes on variable grids. An interesting topic for future is to establish the theoretical analysis for the high-order schemes (e.g., WSBDF3 method) on variable grids.

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