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UNCONDITIONALLY OPTIMAL ERROR ESTIMATE OF A LINEARIZED VARIABLE-TIME-STEP BDF2 SCHEME FOR NONLINEAR PARABOLIC EQUATIONS*

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Abstract. In this paper we consider a linearized variable-time-step two-step backward differentiation formula (BDF2) scheme for solving nonlinear parabolic equations. The scheme is constructed by using the variable time-step BDF2 for the linear term and a Newton linearized method for the nonlinear term in time combining with a Galerkin finite element method (FEM) in space. We prove the unconditionally optimal error estimate of the proposed scheme under mild restrictions on the ratio of adjacent time-steps, i.e. the ratio less than 4.8645, and on the maximum time step. The proof involves the discrete orthogonal convolution (DOC) and discrete complementary convolution (DCC) kernels, and the error splitting approach. In addition, our analysis also shows that the first level solution obtained by BDF1 (i.e. backward Euler scheme) does not cause the loss of global accuracy of second order. Numerical examples are provided to demonstrate our theoretical results.

Keywords. Nonlinear parabolic equations; variable time-step BDF2; orthogonal convolution kernels; stability and convergence; error splitting approach.

AMS subject classifications. 65M06; 65M12.

1. Introduction

In this paper, we focus on the unconditionally optimal error estimate of a linearized second-order two-step backward differentiation formula (BDF2) scheme with variable time steps for solving the following general nonlinear parabolic equation [5, 26]:

$$\begin{aligned} &\partial_t u = \Delta u + f(u), && \boldsymbol{x}\in\Omega, t\in(0,T],\\ &u(\boldsymbol{x},0)=u_0(\boldsymbol{x}), && \boldsymbol{x}\in\Omega,\\ &u(\boldsymbol{x},t)=0, && \boldsymbol{x}\in\partial\Omega, t\in[0,T], \end{aligned} \tag{1.1}$$

where $\Omega\subset\mathbb{R}^d (d=1,2,3)$ is a bounded convex domain. To construct variable time-step schemes, we first set the variable time levels $0=t_0<t_1<\cdots<t_N=T$, the k-th time-step size $\tau_k \overset{\text{def}}{=} t_k - t_{k-1}$, the maximum step size $\tau \overset{\text{def}}{=} \max_{1\le k\le N}\tau_k$, and the adjacent time-step ratios $r_k=\tau_k/\tau_{k-1}$, $2\le k\le N$. Set $u^k=u(t_k), \nabla_\tau u^k \overset{\text{def}}{=} u^k-u^{k-1}$, $r_1\equiv 0$, and denote U^n as the approximation of the exact solution $u(t_n)$. The first step value U^1 is calculated by one-step backward difference formula (BDF1), and the other U^n $(n>1)$ is calculated by BDF2 formula with variable time steps, which are respectively given as

$$\mathcal{D}_1 U^1 = \frac{1}{\tau_1}\nabla_\tau U^1, \quad \mathcal{D}_2 U^n = \frac{1+2r_n}{\tau_n(1+r_n)}\nabla_\tau U^n - \frac{r_n^2}{\tau_n(1+r_n)}\nabla_\tau U^{n-1}. \tag{1.2}$$

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The nonlinear term is approximated by a linearized method, i.e., the Newton linearized method given as

$$f(u^n) \approx f(U^{n-1}) + f'(U^{n-1})\nabla_\tau U^n. \tag{1.3}$$

Thus the semi-discrete BDF2 scheme with variable time steps to problem (1.1) is given as

$$\mathcal{D}_2 U^n = \Delta U^n + f(U^{n-1}) + f'(U^{n-1})\nabla_\tau U^n, \qquad \text{for} \quad 1 \le n \le N, \tag{1.4}$$

$$U^0(\boldsymbol{x}) = u_0(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \tag{1.5}$$

$$U^n(\boldsymbol{x}) = 0, \qquad \boldsymbol{x} \in \partial\Omega, \quad n = 0, 1, \cdots, N. \tag{1.6}$$

Here the BDF1 and BDF2 formulas have been written as a unified convolution form of

$$\mathcal{D}_2 U^n = \sum_{k=1}^{n} b_{n-k}^{(n)} \nabla_\tau U^k, \qquad n \ge 1 \tag{1.7}$$

by taking $b_0^{(n)} = (1+2r_n)/(\tau_n(1+r_n))$, $b_1^{(n)} = -r_n^2/(\tau_n(1+r_n))$ and $b_j^{(n)} = 0$ for $2 \le j \le n-1$.

For the spatial discretization, let $\mathcal{I}_h$ be the quasiuniform partition of Ω with triangles in $\mathbb{R}^2$ or tetrahedra T_i $(i = 1, \cdots, M)$ in $\mathbb{R}^3$, see [12, 23]. Denote the spatial mesh size by $h = \max_{1 \le i \le M}\{\text{diam } T_i\}$ and the finite-dimensional subspace of $H_0^1(\Omega)$ by V_h which consists of piecewise polynomials of degree r $(r \ge 1)$ on $\mathcal{I}_h$. Then, the Newton linearized Galerkin FEM BDF2 scheme with variable time steps is to find $U_h^n \in V_h$ such that

$$(\mathcal{D}_2 U_h^n, v_h) = -(\nabla U_h^n, \nabla v_h) + (f(U_h^{n-1}) + f'(U_h^{n-1})\nabla_\tau U_h^n, v_h), \quad \forall v_h \in V_h. \tag{1.8}$$

Efficiency, accuracy and reliability are of key considerations in numerical analysis and scientific computing. For the time-dependent models appearing in science and engineering, a heuristic and promising method to improve efficiency without sacrificing accuracy is the time adaptive method. For instance, one may employ the coarse-grained or refined time steps based on the solutions changing slowly or rapidly to capture the dynamics of the solutions. One can refer to [17, 18] for phase field models and for blow-up problems [20]. Another alternative approach is to employ high-order methods in time to have the same accuracy with a relatively large time-step. In this paper, we consider the second order BDF2 scheme with variable time steps.

Due to its nice property (A-stable), the BDF2 method with variable time steps has been widely used in various models to obtain computationally efficient, accurate results [3, 15–17, 24, 28]. Much works have been carried out on its stability and error estimates [1–4, 6, 19, 22, 25, 27], but the analysis even for linear parabolic problems (i.e., problem (1.1) with $f(u) = 0$) is already highly nontrivial and challenging as documented in the classic book [23, Chapter 10]. One also refers to the details in [6–9, 21]. In particular, with the energy method and under a ratio condition $0 < r_k \le 1.868$, Becker [1] presents that the variable time-step BDF2 scheme for a linear parabolic problems is zero-stable. After that, Emmrich [4] gives a similar result with $0 < r_k \le 1.91$. Recently, a promising work in [3] introduce a novel generalized discrete Grönwall-type inequality for the Cahn-Hilliard equation to obtain an energy stability with $0 < r_k \le 3.561$. The works in [19, 27] consider linear parabolic equations based on DOC kernels under $0 \le r_k \le 3.561$ [19] and $0 < r_k \le 4.8645$ [27], respectively. In addition, the robust second-order convergence is further analyzed in [27]. The robustness here means the optimal second-order accuracy holds valid only requiring the time-step sizes $0 < r_k \le 4.8645$.

For the variable-time-step BDF2 method applied to nonlinear parabolic equations, there has been a great progress on the error estimates for the Cahn-Hilliard equation [3], molecular beam epitaxial model without slope selection [16, 28], phase field crystal model [15], and references therein. Among all the numerical methods in [3, 15, 16, 28], the implicit schemes are utilized to deal with the nonlinear terms. Although the implicit schemes are unconditionally stable, they need to solve a nonlinear algebraic system in each time level. To circumvent the extra computational cost for iteratively solving the nonlinear algebraic system, a popular approach is to employ the linearized methods to approximate the nonlinear terms. Combining the variable-time-step BDF2 for linear terms with a linearized method for nonlinear terms, it is natural to ask if the proposed implicit-explicit schemes still remain unconditionally stable. In addition, the focus of this paper is on the general nonlinearity f, which also brings the extra analysis difficulty comparing with the phase-fields models studied in [3, 15, 16, 28], since the good property of the energy dissipation for the phase-fields models does not hold any more for general nonlinearity.

In this paper, we aim to address the unconditionally optimal error estimate $\mathcal{O}(\tau^2 + h^{r+1})$ of the linearized scheme (1.8) in the sense of L^2-norm under the following two conditions:

- **A1** : $0 < r_k \le r_{\max} - \delta$ for any small constant $0 < \delta < r_{\max} \approx 4.8645$ and $2 \le k \le N$, where $r_{\max} = \frac{1}{6}\left(\sqrt[3]{1196 - 12\sqrt{177}} + \sqrt[3]{1196 + 12\sqrt{177}}\right) + \frac{4}{3}$ is the root of equation $x^3 = (1+2x)^2$;
- **A2** : there exists a constant $\hat{C}$ independent of τ and N such that the maximum time step size τ satisfies $\tau \le \hat{C}\frac{1}{\sqrt{N}}$.

The proof of the error estimate is established by the introduction of the temporal-spatial error splitting approach and the concepts of DOC and DCC kernels. The error splitting approach, developed in [11], is used to overcome the unnecessary restrictions of the temporal and spatial mesh sizes. The main idea of the error splitting approach is to first consider the boundedness of $\|U^n\|_{H^2}$ for the solution to semi-discrete Equation (1.4), and then to obtain the estimate of $\|U_h^n\|_{L^\infty}$ for the fully discrete Equation (1.8) by using the following strategy

$$\begin{aligned} \|U_h^n\|_{L^\infty} &\le \|R_h U^n\|_{L^\infty} + \|R_h U^n - U_h^n\|_{L^\infty} \\ &\le C\|U^n\|_{H^2} + Ch^{-d/2}\|R_h U^n - U_h^n\|_{L^2} \\ &\le C + Ch^{-d/2}h^2, \end{aligned} \tag{1.9}$$

where R_h is the projection operator.

The concepts of DOC and DCC kernels, developed in [19, 27], are used to present the stability and convergence analysis under a mild restriction on the ratio of adjacent time-steps, i.e., **A1**. The condition **A1** is the mildest restriction in the current literature, as far as we know, for the variable time-step BDF2 method. On the other hand, due to the usage of a linearized scheme to approximate the general nonlinearity, our optimal error estimate in time suffers from another restriction on the maximum time step, i.e., **A2**. Noting that the condition **A2** only involves the maximum time step, hence it is mild and acceptable/reasonable for the practical simulations to have the convergence order.

For general nonlinearity, our improvements are twofold: (i) comparing with the fully implicit schemes developed [3, 15, 16, 28], a linearized scheme is considered in this paper, and its first rigorous proof of unconditionally optimal convergence is presented under mild restrictions on **A1** and **A2**; (ii) the linearized BDF2 scheme (1.8) still has the second-order accuracy in time as the first-order BDF1 method is used only once to compute the first step value.

The remainder of this paper is organized as follows. In Section 2, we present several important properties of the DOC kernels and DCC kernels which play a key role in our stability and convergence analysis. The unconditional L^∞ boundedness of numerical solutions of the fully discrete scheme is derived in Section 3 and then the unconditionally optimal L^2-norm error estimate is obtained in Section 4. In Section 5, numerical examples are provided to confirm our theoretical analysis.

2. Setting

In this paper, we assume there exists a constant $\mathcal{M}$ such that the solution of problem (1.1) satisfies

$$\begin{aligned}\|u_0\|_{H^{r+1}} + \|u\|_{L^\infty((0,T);H^{r+1})} + \|\partial_t u\|_{L^\infty((0,T);H^{r+1})}\\ + \|\partial_{tt}u\|_{L^\infty((0,T);L^2)} + \|\partial_{ttt}u\|_{L^\infty((0,T);L^2)} \le \mathcal{M},\ r\ge 1.\end{aligned} \tag{2.1}$$

2.1. The properties of DOC and DCC kernels.

We here present the definitions and properties of DCC and DOC kernels, which play crucial roles in our analysis to overcome the difficulties resulting from the variable time steps. The DCC kernels introduced in [10, 13] are defined by

$$\sum_{j=k}^{n} p_{n-j}^{(n)} b_{j-k}^{(j)} \equiv 1, \quad \forall 1\le k\le n,\, 1\le n\le N, \tag{2.2}$$

which satisfy

$$\sum_{j=1}^{n} p_{n-j}^{(n)} \mathcal{D}_2 u^j = \sum_{j=1}^{n} p_{n-j}^{(n)} \sum_{l=1}^{j} b_{j-l}^{(j)} \nabla_\tau u^l = \sum_{l=1}^{n} \nabla_\tau u^l \sum_{j=l}^{n} p_{n-j}^{(n)} b_{j-l}^{(j)} = u^n - u^0, \quad \forall n\ge 1. \tag{2.3}$$

The DOC kernels in [19] are defined by

$$\sum_{j=k}^{n} \theta_{n-j}^{(n)} b_{j-k}^{(j)} = \delta_{nk}, \quad \forall 1\le k\le n,\, 1\le n\le N, \tag{2.4}$$

where the Kronecker delta symbol δ_{nk} holds $\delta_{nk}=1$ if $n=k$ and $\delta_{nk}=0$ if $n\ne k$. By exchanging the summation order, it is straightforward to verify that the DOC kernels satisfy

$$\sum_{j=1}^{n} \theta_{n-j}^{(n)} \mathcal{D}_2 u^j = \sum_{l=1}^{n} \nabla_\tau u^l \sum_{j=l}^{n} \theta_{n-j}^{(n)} b_{j-l}^{(j)} = u^n - u^{n-1}, \quad 1\le n\le N. \tag{2.5}$$

Set $p_{-1}^{(n)} \overset{\text{def}}{=} 0, \forall n\ge 0$. The DCC and DOC kernels have the following relations (see [27, Proposition 2.1])

$$p_{n-j}^{(n)} = \sum_{l=j}^{n} \theta_{l-j}^{(l)}, \quad \theta_{n-j}^{(n)} = p_{n-j}^{(n)} - p_{n-1-j}^{(n-1)}, \quad \forall 1\le j\le n. \tag{2.6}$$

We now present several useful lemmas with details in [19, 27, 28].

LEMMA 2.1 ([28]). *Assume the time step ratio r_k satisfies* **A1**. *For any real sequence $\{w_k\}_{k=1}^n$ and any given small constant $0<\delta<r_{\max}\approx 4.8645$, it holds*

$$2w_k\sum_{j=1}^{k}b_{k-j}^{(k)}w_j \geq \frac{r_{k+1}\sqrt{r_{\max}}}{(1+r_{k+1})}\frac{w_k^2}{\tau_k}-\frac{r_k\sqrt{r_{\max}}}{(1+r_k)}\frac{w_{k-1}^2}{\tau_{k-1}}+\frac{\delta w_k^2}{20\tau_k},\quad k\geq 2, \tag{2.7}$$

$$2\sum_{k=1}^{n}w_k\sum_{j=1}^{k}b_{k-j}^{(k)}w_j \geq \frac{\delta}{20}\sum_{k=1}^{n}\frac{w_k^2}{\tau_k}\geq 0,\quad \text{for } n\geq 1. \tag{2.8}$$

COROLLARY 2.1 ([27]). *If the conditions in Lemma 2.1 are satisfied, then we have the following inequality*

$$\sum_{k=1}^{n}w_k\sum_{j=1}^{k}\theta_{k-j}^{(k)}w_j\geq 0,\quad \text{for } n\geq 1. \tag{2.9}$$

LEMMA 2.2 ([19]). *The DOC kernels $\theta_{n-j}^{(n)}$ satisfy*

$$\theta_{n-j}^{(n)}>0 \ \text{ for } 1\leq j\leq n, \qquad \text{and} \qquad \sum_{j=1}^{n}\theta_{n-j}^{(n)}=\tau_n \ \text{ for } n\geq 1. \tag{2.10}$$

PROPOSITION 2.1. ([27, Proposition 2.2]). *The DCC kernels $p_{n-k}^{(n)}$ defined in (2.2) satisfy*

$$\sum_{j=1}^{n}p_{n-j}^{(n)}=\sum_{k=1}^{n}\sum_{j=1}^{k}\theta_{k-j}^{(k)}=t_n,\qquad p_{n-j}^{(n)}\leq 2\tau. \tag{2.11}$$

3. The L^∞ boundedness of the fully discrete solution U_h^n

The key point in this paper, to deal with the nonlinear term in (1.8), is the L^∞ boundedness of the numerical solution U_h^n. To this end, we present several useful lemmas as follows, including the discrete Grönwall inequality and the temporal consistency errors. For convenience, hereafter we denote $\|\cdot\|\overset{\text{def}}{=}\|\cdot\|_{L^2}$.

LEMMA 3.1 (Discrete Grönwall inequality). *Assume $\lambda>0$ and the sequences $\{v_j\}_{j=1}^N$ and $\{\eta_j\}_{j=0}^N$ are nonnegative. If*

$$v_n\leq \lambda\sum_{j=1}^{n-1}\tau_j v_j+\sum_{j=0}^{n}\eta_j,\quad \text{for}\quad 1\leq n\leq N,$$

then it holds

$$v_n\leq \exp\big(\lambda t_{n-1}\big)\sum_{j=0}^{n}\eta^j,\quad \text{for}\quad 1\leq n\leq N.$$

Lemma 3.1 can be proved by the standard induction hypothesis and we omit it here.

LEMMA 3.2 ([14]). *Assume the regularity condition (2.1) holds and the nonlinear function $f=f(u)\in C^2(\mathbb{R})$. Denote the local truncation error by*

$$R_f^j=f(u^j)-f(u^{j-1})-f'(u^{j-1})\nabla_\tau u^j,\quad 1\leq j\leq N. \tag{3.1}$$

Then we have the following estimates of the truncation error

$$\|R_f^j\| \le C_f \tau_j^2, \quad 1 \le j \le N, \tag{3.2}$$

where $C_f \stackrel{\text{def}}{=} \frac{1}{2} C_\Omega \sup_{|u| \le C_\Omega \mathcal{M}} |f''(u)| \mathcal{M}^2$.

LEMMA 3.3. *Assume the regularity condition* (2.1) *holds, the truncation error* $R_t^j = \mathcal{D}_2 u(t_j) - \partial_t u(t_j)\,(1 \le j \le N)$ *has the properties:*

$$\|R_t^1\| \le \frac{\mathcal{M}}{2}\tau_1, \quad \|R_t^j\| \le \frac{3}{2}\mathcal{M}\tau_j\tau, \quad 2 \le j \le N. \tag{3.3}$$

The proofs of Lemmas 3.2 and 3.3 mainly use the Taylor expansion, and are left to Appendix A and Appendix B for brevity.

3.1. Analysis of a semi-discrete scheme. As indicated in (1.9), we first consider the boundedness of the solution to semi-discrete scheme (1.4) in this subsection, and leave the boundedness of the error $\|U^n - U_h^n\|_{L^\infty}$ in next subsection.

Let $e^n = u^n - U^n\,(n = 0, 1, \ldots, N)$. Subtracting (1.4) from (1.1), one has

$$\mathcal{D}_2 e^n = \Delta e^n + R_t^n + R_f^n + E_1^n, \tag{3.4}$$

where $E_1^n = f(u^{n-1}) + f'(u^{n-1})\nabla_\tau u^n - f(U^{n-1}) - f'(U^{n-1})\nabla_\tau U^n$.

THEOREM 3.1. *Assume the conditions* **A1** *and* **A2** *and the regularity condition* (2.1) *hold, and the nonlinear function* $f \in C^2(\mathbb{R})$. *Then the semi-discrete system (1.4) has a unique solution* U^n. *Moreover, there exists an* $\tau^{**} > 0$ *such that the following estimates hold for all* $\tau \le \tau^{**}$

$$\|e^n\|_{H^1} \le C_1 \tau^{\frac{3}{2}}, \tag{3.5}$$

$$\|U^n\|_{L^\infty} \le C_\Omega \|U^k\|_{H^2} \le C_\Omega(\mathcal{M} + 1), \tag{3.6}$$

$$\sum_{j=1}^{n} \|\nabla_\tau e^j\|_{H^2} \le C_2. \tag{3.7}$$

More precisely, in (3.5), we have $\|e^n\| \le C_3 \tau^2$ *and* $\|\nabla e^n\| \le C_4 \tau^{\frac{3}{2}}$, *where* $C_i\,(i = 1, 2, 3, 4)$ *are positive constants independent of* τ.

Proof. Set

$$\tau^{**} = \min\{1, 1/(8C_5), 1/C_8\}, \tag{3.8}$$

where C_5, C_8 will be determined later. Noting that, at each time level, (1.4) is a linear elliptic problem, it is easy to obtain the existence and uniqueness of solution U^n. We use here mathematical induction to prove (3.5) and (3.6), which obviously hold for the initial level $n = 0$. Assume (3.5) and (3.6) hold for $0 \le n \le k-1\,(k \le N)$. Based on the boundedness of $\|U^{n-1}\|_{L^\infty}$ and $\|u^{n-1}\|_{L^\infty}$ for $1 \le n \le k$, we have

$$\begin{aligned} \|E_1^n\| &= \|f(u^{n-1}) + f'(u^{n-1})\nabla_\tau u^n - (f(U^{n-1}) + f'(U^{n-1})\nabla_\tau U^n)\| \\ &\le \|f(u^{n-1}) - f(U^{n-1})\| + \|(f'(u^{n-1}) - f'(U^{n-1}))u^n\| + \|f'(U^{n-1})(u^n - U^n)\| \\ &\quad + \|(f'(u^{n-1}) - f'(U^{n-1}))u^{n-1}\| + \|f'(U^{n-1})(u^{n-1} - U^{n-1})\| \\ &\le C_5(\|e^{n-1}\| + \|e^n\|), \end{aligned} \tag{3.9}$$

where $C_5 = 2\sup_{|v|\le C_\Omega(\mathcal{M}+1)}|f'(v)| + 2C_\Omega\mathcal{M}\sup_{|v|\le C_\Omega(\mathcal{M}+1)}|f''(v)|$.

We now prove that (3.5) and (3.6) hold at $n=k$. Set $n=j$ in (3.4). Multiplying $\theta_{l-j}^{(l)}$ to both sides of (3.4), and summing the resulting from 1 to l, we have

$$\nabla_\tau e^l = \sum_{j=1}^{l}\theta_{l-j}^{(l)}(\Delta e^j + E_1^j) + \sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j), \tag{3.10}$$

where the property of DOC kernels (2.5) is used. Then taking the inner product with e^l on both sides of (3.10), and summing the resulting equality from 1 to k, one has

$$\sum_{l=1}^{k}(\nabla_\tau e^l, e^l) = \sum_{l=1}^{k}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\Delta e^j + E_1^j, e^l) + \sum_{l=1}^{k}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j, e^l). \tag{3.11}$$

Applying (2.8), integration by parts and the inequality $2(a-b)a \ge a^2 - b^2$ to (3.11), we have

$$\begin{aligned}\|e^k\|^2 - \|e^0\|^2 &\le 2\sum_{l=1}^{k}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(E_1^j, e^l) + 2\sum_{l=1}^{k}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j, e^l)\\ &\le 2\sum_{l=1}^{k}\|e^l\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}\|E_1^j\| + 2\sum_{l=1}^{k}\|e^l\|\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j)\|,\end{aligned}$$

which together with the inequality (3.9) and $\|e^0\| = 0$ produces

$$\|e^k\|^2 \le 2C_5\sum_{l=1}^{k}\|e^l\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|e^j\| + \|e^{j-1}\|) + 2\sum_{l=1}^{k}\|e^l\|\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j)\|. \tag{3.12}$$

Choosing an integer $k^*(0\le k^*\le k)$ such that $\|e^{k^*}\| = \max_{0\le i\le k}\|e^i\|$, then the inequality (3.12) yields

$$\begin{aligned}\|e^k\|\|e^{k^*}\| \le \|e^{k^*}\|^2 &\le 4C_5\|e^{k^*}\|\sum_{l=1}^{k^*}\tau_l\|e^l\| + 2\|e^{k^*}\|\sum_{l=1}^{k^*}\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j)\|\\ &\le 4C_5\|e^{k^*}\|\sum_{l=1}^{k}\tau_l\|e^l\| + 2\|e^{k^*}\|\sum_{l=1}^{k}\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j)\|,\end{aligned} \tag{3.13}$$

where (2.10) is used. Thus, we arrive at

$$\|e^k\| \le 4C_5\sum_{l=1}^{k}\tau_l\|e^l\| + 2\sum_{l=1}^{k}\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j)\|. \tag{3.14}$$

It follows from (3.8) that

$$\|e^k\| \le 8C_5\sum_{l=1}^{k-1}\tau_l\|e^l\| + 4\sum_{l=1}^{k}\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j)\|. \tag{3.15}$$

According to Proposition 2.1 and Lemmas 2.2, 3.1, 3.2 and 3.3, it holds

$$\|e^k\| \le 4\exp(8C_5 t_{k-1})\Big(\sum_{l=1}^{k}\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j)\|\Big)$$

$$\begin{aligned}
&\leq 4\exp(8C_5 t_{k-1})\Big(\sum_{j=1}^{k} p_{k-j}^{(k)}\|R_f^j\| + \sum_{j=2}^{k} p_{k-j}^{(k)}\|R_t^j\| + p_{k-1}^{(k)}\|R_t^1\|\Big)\\
&\leq 4\mathcal{M}\exp(8C_5 T)\Big(C_f T + \frac{3}{2}\mathcal{M}T + \mathcal{M}\Big)\tau^2 \stackrel{\text{def}}{=} C_3\tau^2. \qquad (3.16)
\end{aligned}$$

Similarly, set $n = l$ in (3.4) and taking inner product with $\nabla_\tau e^l$ on both sides of (3.4), one has

$$\begin{aligned}
(\mathcal{D}_2 e^l, \nabla_\tau e^l) &= (\Delta e^l, \nabla_\tau e^l) + (R_t^l + R_f^l + E_1^l, \nabla_\tau e^l)\\
&= -(\nabla e^l, \nabla_\tau \nabla e^l) + (R_t^l + R_f^l + E_1^l, \nabla_\tau e^l). \qquad (3.17)
\end{aligned}$$

Summing l from 1 to k on (3.17), using (2.8) and the identity $2a(a-b) = a^2 - b^2 + (a-b)^2$, we have

$$\frac{\delta}{20}\sum_{l=1}^{k}\frac{\|\nabla_\tau e^l\|}{\tau_l} + \|\nabla e^k\|^2 - \|\nabla e^0\|^2 + \sum_{l=1}^{k}\|\nabla_\tau \nabla e^l\|^2 \leq 2\sum_{l=1}^{k}(R_t^l + R_f^l + E_1^l, \nabla_\tau e^l). \qquad (3.18)$$

It follows from Young's inequality that

$$2\sum_{l=1}^{k}(R_t^l + R_f^l + E_1^l, \nabla_\tau e^l) \leq \sum_{l=1}^{k}\Big(\frac{\delta}{20}\frac{\|\nabla_\tau e^l\|^2}{\tau_l} + \frac{20\tau_l}{\delta}\|R_t^l + R_f^l + E_1^l\|^2\Big). \qquad (3.19)$$

Applying (3.19) and $\nabla e^0 = 0$ to (3.18), we arrive at

$$\begin{aligned}
\|\nabla e^k\|^2 + \sum_{l=1}^{k}\|\nabla_\tau \nabla e^l\|^2 &\leq \frac{20}{\delta}\sum_{l=1}^{k}\tau_l\|R_t^l + R_f^l + E_1^l\|^2\\
&\leq \frac{60}{\delta}\Big(\tau_1\|R_t^1\|^2 + \sum_{l=2}^{k}\tau_l\|R_t^l\|^2 + \sum_{l=1}^{k}\tau_l(\|R_f^l\|^2 + \|E_1^l\|^2)\Big). \qquad (3.20)
\end{aligned}$$

Applying the estimates (3.9) and (3.16), Lemmas 3.2 and 3.3 to the inequality (3.20), one yields

$$\begin{aligned}
\|\nabla e^k\|^2 + \sum_{l=1}^{k}\|\nabla_\tau \nabla e^l\|^2 &\leq \frac{60}{\delta}\tau^3\Big(\frac{\mathcal{M}^2}{4} + \frac{9}{4}\mathcal{M}^2 T\tau + TC_f^2\tau + 2TC_5^2C_3^2\tau\Big)\\
&\leq \frac{60}{\delta}\tau^3\Big(\frac{\mathcal{M}^2}{4} + \frac{9}{4}\mathcal{M}^2 T + TC_f^2 + 2TC_5^2C_3^2\Big) \stackrel{\text{def}}{=} C_4^2\tau^3, \qquad (3.21)
\end{aligned}$$

where $\tau \leq 1$ in (3.8) is used. Thus, the estimates (3.21) and (3.16) yield the following H^1 norm estimate

$$\|e^k\|_{H^1} \leq \sqrt{C_3^2 + C_4^2}\,\tau^{\frac{3}{2}} \stackrel{\text{def}}{=} C_1\tau^{\frac{3}{2}}. \qquad (3.22)$$

In the remainder, we will prove $\|U^k\|_{L^\infty} \leq C_\Omega(\mathcal{M}+1)$. To do so, we need to estimate $\|\Delta e^k\|$ due to the facts that $|e^k|_2 \leq \tilde{C}\|\Delta e^k\|$ (here $|\cdot|_2$ denote the semi-norm of H^2-norm) and

$$\|U^k\|_{L^\infty} \leq \|u^k\|_{L^\infty} + \|e^k\|_{L^\infty} \leq C_\Omega\mathcal{M} + C_\Omega\|e^k\|_{H^2}, \qquad (3.23)$$

where the embedding theorem is used in the last inequality. We now consider the estimate of $\|\Delta e^k\|$ by taking inner product with $-\nabla_\tau \Delta e^l$ on both sides of (3.4) (set $n=l$), and have

$$(\mathcal{D}_2 \nabla e^l, \nabla_\tau \nabla e^l) + (\Delta e^l, \nabla_\tau \Delta e^l) = (R_t^l + R_f^l + E_1^l, -\nabla_\tau \Delta e^l). \tag{3.24}$$

Summing l from 1 to k on (3.24), using $2(a-b)a = a^2 - b^2 + (a-b)^2$, the positiveness (2.8) and $\Delta e^0 = 0$, we have

$$\sum_{l=1}^{k} \|\nabla_\tau \Delta e^l\|^2 + \|\Delta e^k\|^2 \le 2 \sum_{l=1}^{k} \|R_t^l + R_f^l + E_1^l\| \|\nabla_\tau \Delta e^l\|, \tag{3.25}$$

Applying Young's inequality to (3.25), one has

$$\|\Delta e^k\|^2 \le \sum_{l=1}^{k} \|R_t^l + R_f^l + E_1^l\|^2. \tag{3.26}$$

According to (3.9) and (3.16) and Lemmas 3.2 and 3.3, one has

$$\begin{aligned} \sum_{l=1}^{k} \|R_t^l + R_f^l + E_1^l\|^2 &\le 3\big(\|R_t^1\|^2 + \sum_{l=2}^{k} \|R_t^l\|^2 + \sum_{l=1}^{k} (\|R_f^l\|^2 + \|E_1^l\|^2)\big) \\ &\le \big(\frac{3}{4}\mathcal{M}^2 + \frac{27}{4}\mathcal{M}^2 t_k \tau + 3C_f^2 t_k \tau + 3C_5^2 C_3^2 k \tau^2\big)\tau^2 \\ &\le \big(\frac{3}{4}\mathcal{M}^2 + \frac{27}{4}\mathcal{M} T + 3C_f^2 T + 3C_5^2 C_3^2 \hat{C}^2\big)\tau^2 \overset{\text{def}}{=} C_7^2 \tau^2, \end{aligned} \tag{3.27}$$

where one uses the maximum time-step assumption **A2** and (3.8) in the last inequality. Inserting (3.27) into (3.26), we derive

$$\|\Delta e^k\| \le C_7 \tau. \tag{3.28}$$

Thus, from the estimates (3.28) and (3.22), the condition (3.8) and the facts that $|e^k|_2 \le \tilde{C}\|\Delta e^k\|$, we arrive at

$$\|e^k\|_{H^2} \le C_8 \tau, \tag{3.29}$$

where $C_8 = \sqrt{C_1^2 + \tilde{C}^2 C_7^2}$. Thus, combining (3.29), (3.23) and (3.8), one has

$$\|U^k\|_{L^\infty} \le \|u^k\|_{L^\infty} + \|e^k\|_{L^\infty} \le C_\Omega \Big(\mathcal{M} + C_8 \tau\Big) \le C_\Omega (\mathcal{M} + 1). \tag{3.30}$$

Therefore, (3.5) and (3.6) hold for $n=k$, i.e., the estimates (3.5) and (3.6) are proved.

The last claim (3.7) can be proved based on the result (3.30). With the help of Cauchy inequality, from (3.16) and (3.21) and the fact $|\nabla_\tau e^l|_2 \le \tilde{C}\|\nabla_\tau \Delta e^l\|$, we have

$$\begin{aligned} \big(\sum_{l=1}^{n} \|\nabla_\tau e^l\|_{H^2}\big)^2 &\le n \sum_{l=1}^{n} \|\nabla_\tau e^l\|_{H^2}^2 \le n \sum_{l=1}^{n} \|\nabla_\tau e^l\|^2 + n \sum_{l=1}^{n} \|\nabla_\tau \nabla e^l\|^2 + n\tilde{C}^2 \sum_{l=1}^{n} \|\nabla_\tau \Delta e^l\|^2 \\ &\le 4C_3^2 N^2 \tau^4 + N C_4^2 \tau^3 + N\tilde{C}^2 \sum_{l=1}^{n} \|\nabla_\tau \Delta e^l\|^2. \end{aligned} \tag{3.31}$$

We now estimate $\sum_{l=1}^{n}\|\nabla_\tau\Delta e^l\|^2$. Applying Young's inequality $2ab\le 8a^2+\frac{1}{2}b^2$ and inequality (3.27) to (3.25), one has

$$\sum_{l=1}^{k}\|\nabla_\tau\Delta e^k\|^2\le 16\sum_{l=1}^{k}\|R_t^l+R_f^l+E_1^l\|^2\le C_7^2\tau^2. \tag{3.32}$$

Inserting (3.32) into (3.31), then it follows from the condition **A2** and (3.8) that

$$\Big(\sum_{l=1}^{n}\|\nabla_\tau e^l\|_{H^2}\Big)^2\le 4C_3^2\hat{C}^4+C_4^2\hat{C}^2+C_7^2\tilde{C}^2\hat{C}^2\overset{\text{def}}{=}C_2^2.$$

The proof is completed. ∎

REMARK 3.1. The condition **A2** is needed in the estimates of Δe^n and $\sum_{l=1}^{n}\|\nabla_\tau e^l\|_{H^2}$ such that $N\tau^2=\mathcal{O}(1)$. The condition **A2**, arising from the proof of the boundedness of $\|U_h^n\|_{L^\infty}$ in Theorem 3.1, may be only sufficient but unnecessary to achieve the optimal unconditional error estimate. It's easy for one to find that, if the nonlinear function $f(\cdot)$ is globally Lipschitz continuous, i.e., there exists a constant L such that $|f(x_1)-f(x_2)|\le L|x_1-x_2|,\forall x_1,x_2\in\mathbb{R}$, the boundedness of $\|U_h^n\|_{L^\infty}$ is redundant in the numerical analysis, and then the condition **A2** will be not required. Another example, if the nonlinear function $f(\cdot)$ is taken such that the Equation (1.1) admits an energy dissipation law (such as the phase field models [3, 15, 16, 28]), then $\|U_h^n\|_{L^\infty}$ can be bounded by a (modified) discrete energy. In this situation, it is also possible to remove **A2** in the proof. But for the general nonlinearity, it is hard to figure out if the condition **A2** is necessary or not, and the further study is worthy of exploring in the future. For now, the ratio restriction **A2** is closely related to the spatio-temporal error splitting approach, which is used to handle the general nonlinearity, and is by far the weakest condition we need to conduct our analysis. If we expect to have the optimal second-order convergence without the condition **A2**, we may need to apply other techniques instead of the spatio-temporal error splitting approach, or to give more refined estimates to circumvent the term of $N\tau^2$, such as using the form of $t_n\tau$. The refined estimate is very complicated, and hence, the research on **A2** condition is still open and worthy of further study. Besides, the condition **A2** is mild and reasonable when one expects to have the optimal second-order convergence.

3.2. Analysis of the fully discrete scheme. We now consider the boundedness of the fully discrete solution U_h^n, which plays the key role of the proof of Theorem 4.1. Define the Ritz projection operator $R_h:H_0^1(\Omega)\to V_h\subseteq H_0^1(\Omega)$ by

$$(\nabla(v-R_hv),\nabla\omega)=0,\quad \forall\omega\in V_h. \tag{3.33}$$

The Ritz projection R_h has the following estimate (for example, see [23, Lemma 1.1])

$$\|v-R_hv\|+h\|\nabla(v-R_hv)\|\le C_\Omega h^s\|v\|_{H^s},\quad \forall v\in H^s(\Omega)\cap H_0^1(\Omega),1\le s\le r+1. \tag{3.34}$$

Thanks to the boundedness of the semi-discrete solutions and (1.9), we only need to estimate $\|U^n-U_h^n\|_{L^\infty}$, which can be split by the Ritz projection into the following two parts

$$U^n-U_h^n=U^n-R_hU^n+R_hU^n-U_h^n\overset{\text{def}}{=}\eta^n+\xi^n,\quad n=0,1,\dots,N. \tag{3.35}$$

For the projection error η^n, it follows from (3.34) that

$$\|\eta^n\| \le C_\Omega h^s \|U^n\|_{H^s}, \quad 0 \le s \le r+1. \tag{3.36}$$

Thus, in remainder of this subsection, the focus is on the estimate of the second term ξ^n. To do so, we now consider the weak form of the semi-discrete equation (1.4) given as

$$(\mathcal{D}_2 U^n, v_h) = -(\nabla U^n, \nabla v_h) + (f(U^{n-1}) + f'(U^{n-1})\nabla_\tau U^n, v_h), \quad \forall v_h \in H_0^1(\Omega). \tag{3.37}$$

Subtracting (1.8) from (3.37), one can use the orthogonality (3.33) to obtain

$$(\mathcal{D}_2 \xi^n, v_h) = -(\nabla \xi^n, \nabla v_h) - (\mathcal{D}_2 \eta^n, v_h) + (E_2^n, v_h), \quad \forall v_h \in V_h, \tag{3.38}$$

where

$$E_2^n = f(U^{n-1}) + f'(U^{n-1})\nabla_\tau U^n - \Big(f(U_h^{n-1}) + f'(U_h^{n-1})\nabla_\tau U_h^n\Big). \tag{3.39}$$

Let $n=j$ in (3.38). Then, multiplying $\theta_{l-j}^{(l)}$ by (3.38), summing j from 1 to l, and using the property (2.5), one has

$$(\nabla_\tau \xi^l, v_h) = -(\sum_{j=1}^{l} \theta_{l-j}^{(l)} \nabla \xi^j, \nabla v_h) - (\nabla_\tau \eta^l, v_h) + (\sum_{j=1}^{l} \theta_{l-j}^{(l)} E_2^j, v_h). \tag{3.40}$$

THEOREM 3.2. *Assume the semi-discrete scheme (1.4) has a unique solution U^n $(n=1,\ldots,N)$. Then the finite element system defined in (1.8) has a unique solution U_h^n $(n=1,\ldots,N)$, and there exist $\tau^{***} = \min\{\tau^{**}, 1/(8C_{11})\}$ and $h^{**} = (C_{10}C_\Omega)^{-\frac{2}{4-d}}$ such that when $\tau < \tau^{***}$ and $h < h^{**}$, it holds*

$$\|\xi^n\| \le C_{10} h^2, \tag{3.41}$$
$$\|U_h^n\|_{L^\infty} \le Q, \tag{3.42}$$

where $Q = \bar{C}(\mathcal{M}+1)+1$, C_{10}, C_{11}, C_Ω are constants independent of τ.

Proof. It is obvious that the solution U_h^n of (1.8) uniquely exists since the coefficients matrix of (1.8) is diagonally dominant. Similar to the proof of Theorem 3.1, mathematical induction is also used to prove (3.41) and (3.42). At the beginning, it is easy to check $\xi^0 + \eta^0 = U^0 - U_h^0 = 0$ by (3.35), and the inequality (3.41) also holds for $n=0$ according to (3.34). Assume (3.41) holds for all $n \le k-1$. It is known that $\|R_h v\|_{L^\infty} \le \bar{C}\|v\|_{H^2}$ for any $v \in H^2(\Omega)$. Thus, from Theorem 3.1, the projection $R_h U^n$ is bounded in the sense of L^∞-norm, namely

$$\|R_h U^n\|_{L^\infty} \le \bar{C}(\mathcal{M}+1).$$

Together with (3.36), it holds for $n \le k-1$ and $h \le h^{**} = (C_{10}C_\Omega)^{-\frac{2}{4-d}}$ that

$$\begin{aligned} \|U_h^n\|_{L^\infty} &\le \|R_h U^n\|_{L^\infty} + \|\xi^n\|_{L^\infty} \le \|R_h U^n\|_{L^\infty} + C_\Omega h^{-\frac{d}{2}} \|\xi^n\| \\ &\le \|R_h U^n\|_{L^\infty} + C_\Omega C_{10} h^{-\frac{d}{2}} h^2 \le \|R_h U^n\|_{L^\infty} + 1 \le Q. \end{aligned} \tag{3.43}$$

Due to the boundedness of $||U^{k-1}||_{L^\infty}$ and $||U_h^{k-1}||_{L^\infty}$, one has

$$\|E_2^k\| \le \|f(U^{k-1}) + f'(U^{k-1})\nabla_\tau U^k - (f(U_h^{k-1}) + f'(U_h^{k-1})\nabla_\tau U_h^k)\|$$

$$
\begin{aligned}
&\leq \|f(U^{k-1})-f(U_h^{k-1})\|+\|(f'(U^{k-1})-f'(U_h^{k-1}))U^k\|+\|f'(U_h^{k-1})(U^k-U_h^k)\|\\
&\quad +\|(f'(U^{k-1})-f'(U_h^{k-1}))U^{k-1}\|+\|f'(U_h^{k-1})(U^{k-1}-U_h^{k-1})\|\\
&\leq C_{11}(\|U^{k-1}-U_h^{k-1}\|+\|U^k-U_h^k\|)\\
&\leq C_{11}(\|\xi^{k-1}\|+\|\xi^k\|+\|\eta^{k-1}\|+\|\eta^k\|)\\
&\leq C_{11}\Big(\|\xi^{k-1}\|+\|\xi^k\|+2C_\Omega(\mathcal{M}+1)h^2\Big),
\end{aligned}
\tag{3.44}
$$

where one uses (3.36) in the last inequality above, and

$$
C_{11}\stackrel{\text{def}}{=}3\sup_{|v|\leq\max(C_\Omega(\mathcal{M}+1),Q)}|f'(v)|+2C_\Omega(\mathcal{M}+1)\sup_{|v|\leq\max(C_\Omega(\mathcal{M}+1),Q)}|f''(v)|.
$$

Taking $v_h=\xi^l$ in (3.40) and summing l from 1 to k, one has

$$
\begin{aligned}
\sum_{l=1}^{k}(\nabla_\tau\xi^l,\xi^l)&=-\sum_{l=1}^{k}(\sum_{j=1}^{l}\theta_{l-j}^{(l)}\nabla\xi^j,\nabla\xi^l)-\sum_{l=1}^{k}(\nabla_\tau\eta^j,\xi^l)+\sum_{l=1}^{k}(\sum_{j=1}^{l}\theta_{l-j}^{(l)}E_2^j,\xi^l)\\
&\leq\sum_{l=1}^{k}\|\xi^l\|\|\nabla_\tau\eta^l\|+\sum_{l=1}^{k}\|\xi^l\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}\|E_2^j\|,
\end{aligned}
\tag{3.45}
$$

where the last inequality uses the positive definiteness of (2.8). Inserting (3.44) into (3.45), one has

$$
\|\xi^k\|^2\leq\|\xi^0\|^2+2\sum_{l=1}^{k}\|\xi^l\|\|\nabla_\tau\eta^l\|+2C_{11}\sum_{l=1}^{k}\|\xi^l\|\sum_{j=1}^{l}\theta_{l-j}^{(l)}\Big(\|\xi^{j-1}\|+\|\xi^j\|+2C_\Omega(\mathcal{M}+1)h^2\Big).
$$

Choosing $k^*(0\leq k^*\leq k)$ such that $\|\xi^{k^*}\|=\max_{0\leq i\leq k}\|\xi^i\|$. Then the above inequality combined with (2.10) yield

$$
\|\xi^{k^*}\|^2\leq\|\xi^0\|\|\xi^{k^*}\|+2\|\xi^{k^*}\|\sum_{l=1}^{k^*}\|\nabla_\tau\eta^l\|+4C_{11}\|\xi^{k^*}\|\Big(C_\Omega(\mathcal{M}+1)Th^2+\sum_{l=1}^{k^*}\tau_l\|\xi^l\|\Big).
$$

Thus, one further has

$$
\|\xi^k\|\leq\|\xi^0\|+2\sum_{l=1}^{k}\|\nabla_\tau\eta^l\|+4C_{11}\Big(C_\Omega(\mathcal{M}+1)Th^2+\sum_{l=1}^{k}\tau_l\|\xi^l\|\Big).
$$

According to (3.36) and (3.7), we find

$$
\begin{aligned}
\|\xi^k\|&\leq C_\Omega h^2\|u^0\|_{H^2}+2C_\Omega h^2\sum_{l=1}^{k}\|\nabla_\tau U^l\|_{H^2}+4C_{11}\Big(C_\Omega(\mathcal{M}+1)Th^2+\sum_{l=1}^{k}\tau_l\|\xi^l\|\Big)\\
&\leq(\mathcal{M}+2\sum_{l=1}^{k}(\|\nabla_\tau u^l\|_{H^2}+\|\nabla_\tau e^l\|_{H^2}))C_\Omega h^2+4C_{11}\Big((\mathcal{M}+1)TC_\Omega h^2+\sum_{l=1}^{k}\tau_l\|\xi^l\|\Big)\\
&\leq\Big(\mathcal{M}+2(\mathcal{M}T+C_2+4C_{11}(\mathcal{M}+1)T)\Big)C_\Omega h^2+4C_{11}\sum_{l=1}^{k}\tau_l\|\xi^l\|\\
&\stackrel{\text{def}}{=}C_{12}h^2+4C_{11}\sum_{l=1}^{k}\tau_l\|\xi^l\|,
\end{aligned}
\tag{3.46}
$$

where $\|\xi^0\| = \|R_h U^0 - U_h^0\| = \|R_h u^0 - u^0\| \le C_\Omega h^2 \|u^0\|_{H^2}$ is used. Noting $\tau \le \tau^{***} \le 1/(8C_{11})$, we have

$$\|\xi^k\| \le 2C_{12}h^2 + 8C_{11}\sum_{l=1}^{k-1}\tau_l \|\xi^l\|.$$

Thus, from Lemma 3.1, we arrive at

$$\|\xi^k\| \le 2\exp(8C_{11}T)C_{12}h^2 \stackrel{\text{def}}{=} C_{10}h^2.$$

Hence, for $h \le h^{**}$, it holds

$$\|U_h^k\|_{L^\infty} \le \|R_h U^k\|_{L^\infty} + \|\xi^k\|_{L^\infty} \le \|R_h U^k\|_{L^\infty} + C_\Omega h^{-\frac{d}{2}}\|\xi^k\| \le Q. \tag{3.47}$$

Therefore, the estimates (3.41) and (3.42) hold for $n = k$ and the proof is completed. □

4. Unconditionally optimal L^2-norm error estimate

We now present the unconditionally optimal L^2-norm error estimate for fully discrete scheme (1.8).

THEOREM 4.1.
Assume $u(\cdot,t) \in H^{r+1}(\Omega)\bigcap H_0^1(\Omega)$ for any $t \ge 0$ and $r \ge 1$, and the conditions **A1** *and* **A2** *hold. Then there exist constants τ^* and h^* such that, when $\tau < \tau^*$ and $h < h^*$, the r-degree finite element system defined in (1.8) owns a unique solution and satisfies*

$$\|u^n - U_h^n\| \le C_0^*(\tau^2 + h^{r+1}), \tag{4.1}$$

where C_0^* is a positive constant independent of h and τ.

Proof. The error of fully discrete solution and exact solution can be split into the following two parts

$$\|u^n - U_h^n\| \le \|u^n - R_h u^n\| + \|R_h u^n - U_h^n\| := \|\vartheta^n\| + \|\zeta^n\|. \tag{4.2}$$

Note that the projection error ϑ^n can be immediately estimated by (3.34) as follows

$$\|\vartheta^n\| \le C_\Omega h^s \|u^n\|_{H^s}, \quad 0 \le s \le r+1. \tag{4.3}$$

Thus, we only need to consider ζ^n. Subtracting (1.8) from (1.1), we get the error equation of ζ^n

$$(\mathcal{D}_2\zeta^n, v_h) = -(\nabla\zeta^n, \nabla v_h) - (\mathcal{D}_2\vartheta^n, v_h) + (E_3^n, v_h) + (R_t^n + R_f^n, v_h), \quad \forall v_h \in V_h, \tag{4.4}$$

where $E_3^n = f(u^{n-1}) + f'(u^{n-1})\nabla_\tau u^n - (f(U_h^{n-1}) + f'(U_h^{n-1})\nabla_\tau U_h^n)$.

Let $n = j$ in (4.4). Multiplying (4.4) by DOC kernels $\theta_{l-j}^{(l)}$ and summing j from 1 to l, one has

$$\begin{aligned}(\nabla_\tau\zeta^l, v_h) = &-(\sum_{j=1}^{l}\theta_{l-j}^{(l)}\nabla\zeta^j, \nabla v_h)\\ &-(\nabla_\tau\vartheta^l, v_h) + (\sum_{j=1}^{l}\theta_{l-j}^{(l)}E_3^j, v_h) + (\sum_{j=1}^{l}\theta_{l-j}^{(l)}(R_t^j + R_f^j), v_h),\end{aligned} \tag{4.5}$$

where the property (2.5) is used. Taking $v_h = \zeta^l$ in (4.5), summing l from 1 to n and using the inequality (3.34) and Corollary 2.1, one has

$$\begin{aligned}\sum_{l=1}^{n}(\nabla_\tau \zeta^l,\zeta^l) &= -\sum_{l=1}^{n}\Big(\sum_{j=1}^{l}\theta_{l-j}^{(l)}\nabla\zeta^j,\nabla\zeta^l\Big)-\sum_{l=1}^{n}(\nabla_\tau\vartheta^l,\zeta^l)+\sum_{l=1}^{n}\Big(\sum_{j=1}^{l}\theta_{l-j}^{(l)}(E_3^j+R_t^j+R_f^j),\zeta^l\Big)\\ &\le \sum_{l=1}^{n}\|\nabla_\tau\vartheta^l\|\|\zeta^l\|+\sum_{l=1}^{n}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|E_3^j\|+\|R_f^j\|+\|R_t^j\|)\|\zeta^l\|. \end{aligned} \tag{4.6}$$

Noting

$$\|\nabla_\tau\vartheta^l\|\le C_\Omega\|\nabla_\tau u^l\|_{H^{r+1}}h^{r+1}\le C_\Omega h^{r+1}\Big\|\int_{t_{l-1}}^{t_l}\partial_t u(s)\,\mathrm{d}s\Big\|_{H^{r+1}}\le C_\Omega\mathcal{M}\tau_l h^{r+1},$$

together with the inequality $2(a-b)a\ge a^2-b^2$, we arrive at

$$\|\zeta^n\|^2\le\|\zeta^0\|^2+2\sum_{l=1}^{n}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|E_3^j\|+\|R_f^j\|+\|R_t^j\|)\|\zeta^l\|+2C_\Omega\mathcal{M}h^{r+1}\sum_{l=1}^{n}\tau_l\|\zeta^l\|. \tag{4.7}$$

Thanks to the boundedness of $\|U_h^n\|_{L^\infty}$ in (3.42), the nonlinear term E_3^n can be estimated by

$$\begin{aligned}\|E_3^n\| &= \|f(u^{n-1})+f'(u^{n-1})\nabla_\tau u^n-(f(U_h^{n-1})+f'(U_h^{n-1})\nabla_\tau U_h^n)\|\\ &\le \|f(u^{n-1})-f(U_h^{n-1})\|+\|(f'(u^{n-1})-f'(U_h^{n-1}))u^n\|+\|f'(U_h^{n-1})(u^n-U_h^n)\|\\ &\quad+\|(f'(u^{n-1})-f'(U_h^{n-1}))u^{n-1}\|+\|f'(U_h^{n-1})(u^{n-1}-U_h^{n-1})\|\\ &\le C_{13}\Big(\|u^{n-1}-U_h^{n-1}\|+\|u^n-U_h^n\|\Big)\\ &\le C_{13}\Big(\|\zeta^{n-1}\|+\|\zeta^n\|+\|\vartheta^{n-1}\|+\|\vartheta^n\|\Big)\\ &\le C_{13}\Big(\|\zeta^{n-1}\|+\|\zeta^n\|+2C_\Omega\mathcal{M}h^{r+1}\Big),\end{aligned} \tag{4.8}$$

where the last inequality holds by (3.34) and

$$C_{13}=2\sup_{|v|<\max\{C_\Omega\mathcal{M},Q\}}|f'(v)|+2\sup_{|v|<\max\{C_\Omega\mathcal{M},Q\}}|f''(v)|C_\Omega\mathcal{M}.$$

Inserting (4.8) into (4.7), one has

$$\begin{aligned}\|\zeta^n\|^2\le&\|\zeta^0\|^2+2C_{13}\sum_{l=1}^{n}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|\zeta^{j-1}\|+\|\zeta^j\|)\|\zeta^l\|\\ &+2\sum_{l=1}^{n}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|R_f^j\|+\|R_t^j\|)\|\zeta^l\|+2C_\Omega\mathcal{M}(1+2C_{13})h^{r+1}\sum_{l=1}^{n}\tau_l\|\zeta^l\|.\end{aligned}$$

Choosing n^* such that $\|\zeta^{n^*}\|=\max_{0\le l\le n}\|\zeta^l\|$. The above inequality yields

$$\|\zeta^{n^*}\|^2\le\|\zeta^0\|\|\zeta^{n^*}\|+4C_{13}\sum_{l=1}^{n^*}\sum_{j=1}^{l}\theta_{l-j}^{(l)}\|\zeta^{n^*}\|\|\zeta^l\|$$

$$+2\sum_{l=1}^{n^*}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|R_f^j\|+\|R_t^j\|)\|\zeta^{n^*}\|+2C_\Omega\mathcal{M}(1+2C_{13})h^{r+1}\sum_{l=1}^{n^*}\tau_l\|\zeta^{n^*}\|.$$

Eliminating a $\|\zeta^{n^*}\|$ from both sides and using the facts that $\|\zeta^n\|\le\|\zeta^{n^*}\|$ and $n^*\le n$, we arrive at

$$\begin{aligned}\|\zeta^n\|&\le\|\zeta^0\|+4C_{13}\sum_{l=1}^{n}\tau_l\|\zeta^l\|+2\sum_{l=1}^{n}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|R_f^j\|+\|R_t^j\|)+2C_\Omega\mathcal{M}(1+2C_{13})t_nh^{r+1}\\&\le4C_{13}\sum_{l=1}^{n}\tau_l\|\zeta^l\|+2\sum_{l=1}^{n}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|R_f^j\|+\|R_t^j\|)+C_\Omega\mathcal{M}(2T+4C_{13}T+1)h^{r+1},\end{aligned}\tag{4.9}$$

where $\|\zeta^0\|=\|R_hu_0-U_h^0\|=\|R_hu_0-u_0\|\le C_\Omega h^{r+1}\|u_0\|_{H^{r+1}}$ is used. By exchanging the order of summation and using identity (2.6), Lemmas 3.2, 3.3 and Proposition 2.1, it holds

$$\begin{aligned}2\sum_{l=1}^{n}\sum_{j=1}^{l}\theta_{l-j}^{(l)}(\|R_f^j\|+\|R_t^j\|)&=2\sum_{j=1}^{n}p_{n-j}^{(n)}(\|R_f^j\|+\|R_t^j\|)\\&=2\sum_{j=1}^{n}p_{n-j}^{(n)}\|R_f^j\|+2\sum_{j=2}^{n}p_{n-j}^{(n)}\|R_t^j\|+p_{n-1}^{(n)}\|R_t^1\|\\&\le(2C_ft_n+3t_n\mathcal{M}+\mathcal{M})\tau^2.\end{aligned}\tag{4.10}$$

Thus, inserting (4.10) into (4.9), for $\tau\le\tau^*\le1/(8C_{13})$, we have

$$\|\zeta^n\|\le8C_{13}\sum_{l=1}^{n-1}\tau_l\|\zeta^l\|+2(2C_fT+3T\mathcal{M}+\mathcal{M})\tau^2+2C_\Omega\mathcal{M}(2T+4C_{13}T+1)h^{r+1},$$

which, together with Lemma 3.1, implies that

$$\begin{aligned}\|\zeta^n\|&\le2\exp(8C_{13}T)\big((2C_fT+3T\mathcal{M}+\mathcal{M})\tau^2+C_\Omega\mathcal{M}(2T+4C_{13}T+1)h^{r+1}\big)\\&\le C_{14}(h^{r+1}+\tau^2),\end{aligned}\tag{4.11}$$

where $C_{14}=2\exp(8C_{13}T)\max\{2C_fT+3T\mathcal{M}+\mathcal{M},C_\Omega\mathcal{M}(2T+4C_{13}T+1)\}$. The proof is completed by inserting (4.3) and (4.11) into (4.2) and setting $C_0^*\overset{\text{def}}{=}C_\Omega\mathcal{M}+C_{14}$. □

5. Numerical examples

We now present two examples to investigate the quantitative accuracy of fully discrete scheme (1.8) from two perspectives: (a) the convergence order of numerical scheme (1.8) in time and space; (b) the unconditional convergence by fixing the spatial size h and refining the temporal size τ. To obtain the variable time steps, we construct the time steps by $\tau_k=T\lambda_k/\Lambda$ for $1\le k\le N$, where $\Lambda=\sum_{k=1}^N\lambda_k$ and λ_k is randomly drawn from the uniform distribution on $(0,1)$. In the simulations, we only use the linear finite element (i.e. $r=1$), and consider the time steps in two cases:

Case (i): the ratios of adjacent time steps satisfy **A1**, i.e., $0<r_k<4.8645$;

Case (ii): the ratios do not satisfy **A1**, i.e., can be taken large randomly.

Example 5.1. We here consider the computation of the following 2D nonlinear parabolic equation

$$\partial_t u = \Delta u + \sqrt{1+u^2} + g(\boldsymbol{x},t).$$

In the simulations, we take the final time $T=1$ and the computational domain $\Omega = (0,1)^2$. As a benchmark solution, we take an exact solution in the form of $u(\boldsymbol{x},t) = (1+t^3)x_1(1-x_1)^2 x_2(1-x_2)^2$, and the source term $g(\boldsymbol{x},t)$ can be calculated accordingly.

Table 5.1 shows the spatial L^2-error by increasing M and fixing $N=10^4$. Tables 5.2 and 5.3 show the temporal L^2-errors by taking $M=N$ and increasing N under Cases (i) and (ii) in above, respectively. From Tables 5.1-5.3, the second order convergence rates can be observed, which agrees with the results in Theorem 4.1. In addition, The left panel in Figure 5.1 plots the L^2-error by fixing N and increasing M, which implies that the error estimate is unconditionally stable since the solution does not blowup for any temporal and spatial ratios.

M	error	order	$r_{\max}$
40	4.2893e-05	–	4.6836
80	8.9895e-06	2.2544	4.8091
160	1.9913e-06	2.1745	4.7541
320	4.6221e-07	2.1071	4.7043

TABLE 5.1. *Errors and spatial convergence orders with $N=10^4$ for Example 5.1.*

N	error	order	$r_{\max}$
120	3.6800e-06	–	4.2785
240	8.3695e-07	2.1365	4.6672
480	1.9795e-07	2.0800	4.1304
960	4.8114e-08	2.0406	4.2979

TABLE 5.2. *Errors and time convergence orders with $0<r_k<4.8645$ for Example 5.1.*

N	error	order	$r_{\max}$
120	3.6533e-06	–	21.6746
240	8.3479e-07	2.1297	24.1472
480	1.9783e-07	2.0772	285.448
960	4.7942e-08	2.0449	792.551

TABLE 5.3. *Errors and time convergence orders with $r_k>0$ for Example 5.1.*

Example 5.2. We now consider Allen-Cahn model with an external force

$$\partial_t u = \Delta u + u - u^3 + g(\boldsymbol{x},t).$$

In the simulations, we take the final time $T=1$ and the computational domain $\Omega = (0,1)^3$. Again, as a benchmark solution, we take an exact solution in the form of $u(\boldsymbol{x},t) = (1+t^3)x_1(1-x_1)^2 x_2(1-x_2)^2 x_3(1-x_3)^2$, and the source term $g(\boldsymbol{x},t)$ can be calculated accordingly.

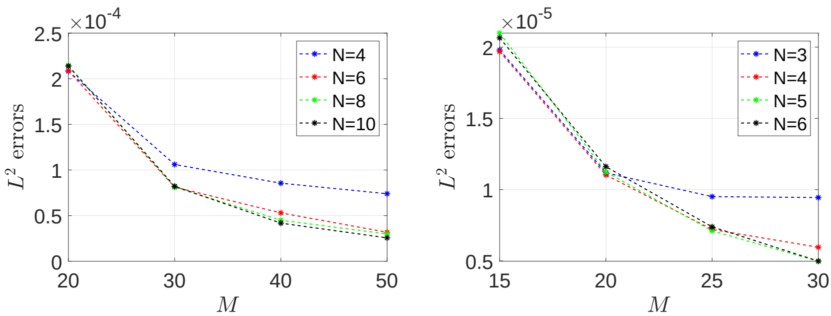

FIG. 5.1. *To investigate the scheme is unconditionally stable, L^2-errors are plotted by increasing M for different given N: left and right panels for Examples 5.1 and 5.2, respectively.*

Table 5.4 shows the spatial L^2-error by increasing M and fixing $N = 10^3$. Tables 5.5 and 5.6 show the temporal L^2-errors by taking $M = N$ and increasing N under Cases (i) and (ii) in above, respectively. From Tables 5.4-5.6, the second-order convergence rates can be observed, which again agrees with the results in Theorem 4.1. The right panel in Figure 5.1 plots the L^2-error by fixing N and increasing M, which again implies that the error estimate is unconditionally stable since the solution does not blowup for any temporal and spatial ratios.

M	error	order	$r_{\max}$
6	1.3595e-04	–	4.5317
12	3.3786e-05	2.0086	4.3782
24	8.4315e-06	2.0025	4.3911
48	2.1069e-06	2.0007	4.6375

TABLE 5.4. *Errors and spatial convergence orders with $N = 10^3$ for Example 5.2.*

N	error	order	$r_{\max}$
4	3.0607e-04	–	2.3893
8	7.5914e-05	2.0114	2.2410
16	1.8918e-05	2.0046	2.9583
32	4.7170e-06	2.0038	3.9028

TABLE 5.5. *Errors and time convergence orders with $0 < r_k < 4.8645$ for Example 5.2.*

N	error	order	$r_{\max}$
4	3.0721e-04	–	2.4017
8	7.5918e-05	2.0167	13.2425
16	1.8929e-05	2.0039	32.1533
32	4.7200e-06	2.0037	25.1107

TABLE 5.6. *Errors and time convergence orders with $r_k > 0$ for Example 5.2.*

6. Conclusions

We have presented the unconditionally optimal error estimate of a linearized variable-time-step BDF2 scheme for nonlinear parabolic equations in conjunction with a Galerkin finite element approximation in space. The rigorous error estimate of $\mathcal{O}(\tau^2+h^{r+1})$ in the L^2-norm has been established under mild assumptions on the ratio of adjacent time steps **A1** and the maximum time-step size **A2**. The analysis is based on the recently developed DOC and DCC kernels and the time-space error splitting approach. The techniques of DOC and DCC kernels facilitate the proof of the second order convergence of BDF2 with a new ratio of adjacent time steps, i.e., $0<r_k<4.8645$. The error splitting approach divides the error estimate of numerical solution into the estimates of $\|U^n\|_{H^2}$ and $\|R_hU^n-U_h^n\|_{L^2}$, which circumvents the ratio restriction of time-space sizes, i.e., this is the so-called unconditionally optimal error estimate.

In addition, our error estimate is robust. The robustness here means the error estimate does not require any extra restriction on time steps except the conditions **A1** and **A2**. Meanwhile, we used the first-order BDF1 to calculate the first level solution u^1, and found that this first-order scheme did not bring the loss of global accuracy of second order. Although great progress has been made for the second-order convergence of variable time-step BDF2 scheme solving nonlinear problems, but most of them use the implicit approximation to the nonlinear terms. As far as we know, it is a pioneering work to present the optimal error estimate for the variable time-step BDF2 scheme with a linearized approximation to nonlinear terms only under the ratio condition $0<r_k<4.8645$ and a mild assumption on maximum time step **A2**. Numerical examples were provided to verify our theoretical analysis.

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Appendix A. The proof of Lemma 3.2.

Proof. **(Proof of Lemma 3.2.)** It follows from the Taylor expansion that

$$\begin{aligned}
\|R_f^j\| &= \|(u^j-u^{j-1})^2\int_0^1 f''(u^{j-1}+s\nabla_\tau u^j)(1-s)\,\mathrm{d}s\| \\
&\le \|u^j-u^{j-1}\|\cdot\|(u^j-u^{j-1})\int_0^1 f''(u^{j-1}+s\nabla_\tau u^j)(1-s)\,\mathrm{d}s\|_{L^\infty} \\
&\le \|\int_{t_{j-1}}^{t_j}\partial_t u\,\mathrm{d}t\|\cdot\|u^j-u^{j-1}\|_{L^\infty}\|\int_0^1 f''(u^{j-1}+s\nabla_\tau u^j)(1-s)\,\mathrm{d}s\|_{L^\infty} \\
&\le \mathcal{M}\tau_j\cdot\|\int_{t_{j-1}}^{t_j}\partial_t u\,\mathrm{d}t\|_{L^\infty}\frac{\sup_{|u|\le C_\Omega\mathcal{M}}|f''(u)|}{2} \\
&\le \frac{1}{2}\mathcal{M}\tau_j\sup_{|u|\le C_\Omega\mathcal{M}}|f''(u)|\int_{t_{j-1}}^{t_j}\|\partial_t u\|_{L^\infty}\,\mathrm{d}t \le \frac{1}{2}\sup_{|u|\le C_\Omega\mathcal{M}}|f''(u)|C_\Omega\mathcal{M}^2\tau_j^2,
\end{aligned}$$

where $\|\partial_t u\|_{L^\infty}\le C_\Omega\|\partial_t u\|_{H^2}\le C_\Omega\mathcal{M}$ is used. The proof is completed. ∎

Appendix B. The proof of Lemma 3.3.

Proof. **(Proof of Lemma 3.3.)** Recall that the first step value u^1 is computed by BDF1, i.e., $R_t^1 = \frac{u_1 - u_0}{\tau_1} - \partial_t u(t_1)$, one has

$$\|R_t^1\| = \|\frac{u_1 - u_0}{\tau_1} - \partial_t u(t_1)\| = \frac{1}{\tau_1}\|\int_0^{t_1} \partial_t u(s) - \partial_t u(t_1)\,\mathrm{d}s\|$$
$$\leq \frac{1}{\tau_1}\int_0^{t_1} \|\partial_t u(s) - \partial_t u(t_1)\|\,\mathrm{d}s \leq \frac{1}{\tau_1}\int_0^{t_1}\int_s^{t_1} \|\partial_{tt} u(t)\|\,\mathrm{d}t\,\mathrm{d}s \leq \frac{\mathcal{M}}{2}\tau_1.$$

For $j \geq 2$, by using the Taylor's expansion formula , one produces (also see [23, Theorem 10.5])

$$R_t^j = -\frac{1+r_j}{2\tau_j}\int_{t_{j-1}}^{t_j} (t - t_{j-1})^2 \partial_{ttt} u\,\mathrm{d}t + \frac{r_j}{2(1+r_j)\tau_{j-1}}\int_{t_{j-2}}^{t_j} (t - t_{j-2})^2 \partial_{ttt} u\,\mathrm{d}t, \quad 2 \leq j \leq N.$$

Combining with the regularity assumption (2.1) and the ratio condition **A1**, one derives

$$\|R_t^j\| \leq \frac{\mathcal{M}}{6}(1+r_j)\tau_j(2\tau_j + \tau_{j-1}) \leq \frac{3}{2}\mathcal{M}\tau_j\tau. \tag{B.1}$$

The proof is completed. ∎

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