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A SECOND ORDER BDF NUMERICAL SCHEME WITH VARIABLE STEPS FOR THE CAHN–HILLIARD EQUATION*

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Abstract. We present and analyze a second order in time variable step BDF2 numerical scheme for the Cahn–Hilliard equation. The construction relies on a second order backward difference, convex-splitting technique and viscous regularizing at the discrete level. We show that the scheme is unconditionally stable and uniquely solvable. In addition, under mild restriction on the ratio of adjacent time-steps, an optimal second order in time convergence rate is established. The proof involves a novel generalized discrete Gronwall-type inequality. As far as we know, this is the first rigorous proof of second order convergence for a variable step BDF2 scheme, even in the linear case, without severe restriction on the ratio of adjacent time-steps. Results of our numerical experiments corroborate our theoretical analysis.

Key words. variable step BDF2 scheme, convergence analysis, Cahn–Hilliard equation

AMS subject classifications. 35K35, 35K55, 65M12, 65M60

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1. Introduction.

Efficiency and accuracy are of central importance in numerical analysis and scientific computing. For a physical/biological/engineering process modeled by a time-dependent PDE, a well-known heuristic method to improve efficiency without sacrificing accuracy is the so-called time adaptive method, where one employs small time-steps when the system is evolving quickly while large time-steps are utilized when the time-evolution is slow [42, 49, 68]. Another approach is to utilize high order in time methods so that relatively large time-steps can be employed for the same error tolerance.

The rigorous numerical analysis of such adaptive methods is relatively easy for one-step methods; see, for instance, [15]. However, the analysis of multistep methods (two or more steps that involve three or more levels) is completely different. For example, in the classical second order backward difference scheme (BDF2), known for its strong stability, the analysis of its variable step version applied to linear parabolic equations is already highly nontrivial and incomplete so far as documented in Chapter 10 of Thomée's classical book [55]. Indeed, the best known result on the variable step

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BDF2 applied to linear parabolic equations only establishes a second order in time convergence rate with a prefactor that blows up at vanishing step sizes for certain choices of time-steps [7, 55]. See Remark 4.1 for more details. See also [11, 26, 27, 37] for relevant work.

For systems whose evolution occurs over a very long time such as the coarsening process associated with the Cahn–Hilliard equation, the long time accuracy or stability is obviously of great importance as well. If the system has an energy law such as the Cahn–Hilliard equation, it is natural to design numerical schemes that inherit the energy law, perhaps in some modified form [28, 50]. This is an example of the so-called memetic methods which usually leads to better results in terms of accuracy and stability. Other examples include a sympletic integrator for Hamiltonian systems [29], a TVD method for hyperbolic conservation laws [17, 53], DRP (dispersion relation preserving) methods for dispersive equations [54], asymptotic preserving methods for kinetic problems [36], and energy/Hamiltonian preserving methods for conservative systems among others. Indeed, it is known that numerical methods that preserve the dissipativity of the underlying dissipative system in some appropriate sense would be able to capture the long-time statistical properties of the dissipative model under approximation [59, 60].

In this paper, we focus on a prototype nonlinear parabolic equation, the Cahn–Hilliard equation, which is a gradient flow (in the H^{-1} norm) whose temporal evolution involves both slow and fast stages, and the coarsening process occurs over a very long time. Therefore, it is highly desirable to develop a variable step BDF2 scheme that is unconditionally stable (and uniquely solvable). We achieve this goal by combining three ideas: variable-step BDF2 for the linear term, convex splitting for the nonlinear term, and a viscous regularization at the discrete level for added stability. The optimal second order in time convergence is established by appropriate combination of energy estimates and a novel generalized discrete Gronwall-type inequality. As far as we know, this is the first time such a second order in time error estimate is proved for variable step BDF2 without severe constraints on the ratio of adjacent time-steps, even for the linear case.

Recall that the classical Ginzburg–Landau energy functional, defined for any $u \in H^1(\Omega)$, is given by (see [10] for a detailed derivation)

$$E(u) = \int_\Omega \left(\frac{1}{4}u^4 - \frac{1}{2}u^2 + \frac{\varepsilon^2}{2}|\nabla u|^2 \right) \mathrm{d}\mathbf{x}, \tag{1.1}$$

where $\varepsilon > 0$ is a parameter that is proportional to the interface width. The Cahn–Hilliard equation is the H^{-1} (conserved) gradient flow of the energy functional (1.1):

$$\begin{cases} u_t = \Delta w \quad \text{in} \quad \Omega \times (0,T), \\ w := \delta_\phi E = u^3 - u - \varepsilon^2 \Delta u \quad \text{in} \quad \Omega \times (0,T), \\ \partial_n u = \partial_n w = 0 \quad \text{on} \quad \partial\Omega \times (0,T), \\ u(\,\cdot\,,0) = u_0 \quad \text{in} \quad \Omega, \end{cases} \tag{1.2}$$

where $T > 0$ is the final time, which may be infinite; $\partial_n u = \boldsymbol{n} \cdot \nabla u$ and $\partial_n w = \boldsymbol{n} \cdot \nabla w$, where $\boldsymbol{n}$ is the unit outward normal vector on the boundary. Due to the gradient structure of (1.2), one can easily derive the following energy dissipation law:

$$\frac{\mathrm{d}}{\mathrm{d}t} E(u(t)) = -\int_\Omega |\nabla w|^2 \mathrm{d}\mathbf{x}. \tag{1.3}$$

In integral form, the energy decay may be expressed as

$$E(u(t_1)) + \int_{t_0}^{t_1} \int_\Omega |\nabla w(t)|^2 d\mathbf{x} dt = E(u(t_0)). \tag{1.4}$$

Furthermore, the equation is mass conservative, i.e., $\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega u \,\mathrm{d}\mathbf{x} = 0$, which follows from the conservative structure of the equation together with the homogeneous Neumann boundary conditions for w. This property can be recast as $(u(\,\cdot\,,t),1) = (u_0,1)$ for all $t \geq 0$, where $(\cdot,\cdot)$ represents the L^2 inner product.

The Cahn–Hilliard equation, which models spinodal decomposition in a binary alloy, is one of the most important models in mathematical physics. The coarsening process associated with the Cahn–Hilliard equation takes a long time (on the order of some positive power of $1/\varepsilon$). It could also couple with other physical/biological processes leading to complex systems such as the Cahn–Hilliard–Navier–Stokes (CHNS) equation (for two-phase flow), the Cahn–Hilliard–Hele–Shaw (CHHS) equation (binary fluid in a Hele-Shaw cell), etc.

Due to the importance of the Cahn–Hilliard model, there is long list of works on the numerical analysis of Cahn–Hilliard. See, for instance, [2, 4, 22, 23, 24, 25, 30, 31, 35, 42, 45, 46, 47, 48, 62] and the references therein for works on first order in time schemes, and [3, 8, 21, 32, 33, 35, 40, 52, 65] and the references therein for related works on second order in time schemes. Second order in time schemes are desirable since one could increase efficiency without sacrificing accuracy by taking larger time-steps with the same error tolerance. However, the analysis of second order schemes is usually more difficult than those for the first order schemes.

The convex splitting scheme, popularized by David Eyre's work [28], is a well-known approach to constructing numerical schemes that inherit the energy law. This framework treats the convex part of the chemical potential implicitly and the concave part explicitly. This results in schemes that are uniquely solvable and unconditionally energy stable, unconditionally with respect to the time and space step sizes. The convex splitting methodology has been applied to a wide class of gradient flows in recent years, and both first and second order accurate in time algorithms have been developed. For the phase field crystal (PFC) equation and the modified phase field crystal (MPFC) equation see the related works [5, 6, 43, 57, 58, 63, 66]; for epitaxial thin film growth models see [12, 14, 51, 56]; for nonlocal Cahn–Hilliard-type models see [38, 39], and for the CHHS and related models see [13, 18, 19, 34, 61]. It is observed that the splitting could lead to significant numerical errors, especially in the first order case [16]. Therefore, second order energy stable methods are more desirable to reduce error. The interested reader is referred to [3, 8, 20, 21, 35, 40, 41, 44, 52, 64, 65, 67] for some of the recent progress in terms of second order schemes for the Cahn–Hilliard equation. In particular, [67] contains a rigorous second order convergence analysis of a convex splitting scheme together with a viscous regularizing term.

The scheme that we propose in this paper is a variable step version of the one proposed in [67]. For $n \geq 1$, given $u_h^{n-1}, u_h^n \in S_h$, find $u_h^{n+1}, w_h^{n+1} \in S_h$, such that

(1.5)
$$\begin{cases} \frac{1}{\tau_{n+1}}\left(\frac{1+2\gamma_{n+1}}{1+\gamma_{n+1}} u_h^{n+1} - (1+\gamma_{n+1})\, u_h^n + \frac{(\gamma_{n+1})^2}{1+\gamma_{n+1}} u_h^{n-1}, v_h\right) = \left(\nabla w_h^{n+1}, \nabla v_h\right) \quad \forall\, v_h \in S_h, \\ \left(w_h^{n+1}, \phi_h\right) = -\left(\varepsilon^2 \nabla u_h^{n+1}, \nabla \phi_h\right) + \left((1+\gamma_{n+1})\, u_h^n - \gamma_{n+1} u_h^{n-1}, \phi_h\right) \\ \qquad\qquad - \left(\left(u_h^{n+1}\right)^3, \phi_h\right) - A\tau_{n+1}\left(\nabla\left(u_h^{n+1} - u_h^n\right), \nabla\phi_h\right) \quad \forall\, \phi_h \in S_h, \end{cases}$$

where S_h is some appropriate finite element space, $\tau_{n+1} = t_{n+1} - t_n$ is the time step size, and $\gamma_{n+1} = \frac{\tau_{n+1}}{\tau_n}$ is the ratio of the adjacent time-steps. The last term is a second order viscous regularization term at the discrete level.

Our main result is the following discrete energy law and second order error estimates under mild constraint on γ_n: there exists an A_0 such that for any $A \geq A_0$, the numerical scheme (2.6) has the energy-decay property,

$$\mathcal{E}\left(u_h^{n+1}, u_h^n, \tau_{n+1}\right) + (A - A_0)\tau_{n+1} \|\nabla\left(u_h^{n+1} - u_h^n\right)\|^2 \leq \mathcal{E}\left(u_h^n, u_h^{n-1}, \tau_n\right),$$

where $\mathcal{E}\left(u_h^{n+1}, u_h^n, \tau_{n+1}\right)$ is the discrete energy, which is defined in (3.3). Moreover, for any given final time $T = \sum_{n=0}^{N_T} \tau_{n+1} > 0$, the following second order convergence under some additional moderate constraints on γ_n and τ holds:

$$\|e_u^{n+1}\|^2 = \|u^{n+1} - u_h^{n+1}\|^2 \leq C\mathcal{R},$$

where C is a generic positive constant and

$$\mathcal{R} = \mathcal{R}^* + h^{2(q+1)} \|u^{n+1}\|_{H^{q+1}}^2, \tag{1.6}$$

and

$$\begin{aligned}
\mathcal{R}^* = &\sum_{k=1}^{n} \tau_{k+1} \left(\tau_{k+1} + \tau_k\right)^3 \left(\int_{t_{k-1}}^{t_{k+1}} \|\partial_{ttt} u\|^2 \mathrm{d}s + \int_{t_{k-1}}^{t_{k+1}} \|\partial_{tt} u\|^2 \mathrm{d}s\right) \\
&+ \sum_{k=1}^{n} \tau_{k+1}^4 \int_{t_k}^{t_{k+1}} \|\partial_t \Delta u\left(s\right)\|^2 \mathrm{d}s + \tau_1^3 \int_{t_0}^{t_1} \|\partial_{tt} u\left(s\right)\|^2 \mathrm{d}s + \tau_1^3 \int_{t_0}^{t_1} \|\partial_t \Delta u\|^2 \mathrm{d}s \\
&+ h^{2(q+1)} \sum_{k=0}^{n} \tau_{k+1} \left(\|w^{k+1}\|_{H^{q+1}}^2 + \|u^{k+1}\|_{H^{q+1}}^2\right) + h^{2(q+1)} \sum_{k=1}^{n} \int_{t_{k-1}}^{t_{k+1}} \|\partial_t u\|_{H^{q+1}}^2 \mathrm{d}s.
\end{aligned}$$

An earlier convergence result on linear parabolic problems derived by Becker [7] contains a prefactor of the form $\exp(C\Gamma_n)$, where $\Gamma_n = \sum_{k=3}^{n} [\gamma_{k-1} - \gamma_{k+1}]_+$. It is easy to construct variable steps so that $\Gamma_n \to \infty$ as the step size approaches zero. See section 4 for more details. Even in the case of finite Γ_n, this prefactor could be huge—effectively infinity—for moderate values of C and Γ_n due to the nature of the exponential function. Such an undesirable prefactor has been completely removed in this work, with the help of a novel generalized discrete Gronwall-type inequality, even in the nonlinear case that we are working on. We also remark that the method here deviates significantly from the constant time-step case [67], where the authors relied on the G-norm in an essential manner. We also point out that the G-norm method fails in our variable step setting unless we have a sequence of monotonically decreasing time-steps, a case of little interest in applications.

The rest of the article is organized as follows. In section 2 we outline the fully discrete scheme. The energy stability analysis is established in section 3. In section 4 we present the $\ell^\infty(0, T; L^2) \cap \ell^2(0, T; H^1)$ convergence analysis for the scheme. The optimal convergence analysis is contained in section 5. Numerical results corroborating our theoretical analysis are presented in section 6. Concluding remarks are offered at the end.

2. The fully discrete numerical scheme.

We use standard notation for the norms on their respective function spaces. In particular, we denote the standard norms for the Sobolev spaces $W^{m,p}(\Omega)$ by $\|\cdot\|_{m,p}$ (see [1]). We replace $\|\cdot\|_{0,p}$ by $\|\cdot\|_p$, $\|\cdot\|_{0,2} = \|\cdot\|_2$ by $\|\cdot\|$, and $\|\cdot\|_{q,2}$ by $\|\cdot\|_{H^q}$.

The mixed weak formulation of Cahn–Hilliard equation (1.2) is to find $u, w \in L^2(0,T;H^1(\Omega))$, with $u_t \in L^2(0,T;H^{-1}(\Omega))$, satisfying

$$\begin{cases} (u_t, v) + (\nabla w, \nabla v) = 0 \qquad \forall\, v \in H^1(\Omega), \\ (w, \psi) = (u^3 - u, \psi) + \varepsilon^2(\nabla u, \nabla \psi) \qquad \forall\, \psi \in H^1(\Omega), \end{cases} \tag{2.1}$$

for almost every $t \in (0,T]$, where H^{-1} is the dual space of H^1(notice that the H^{-1} space we defined here is different from the standard one which is specified as the dual of H_0^1), and $(\cdot,\cdot)$ represents the L^2 inner product or the duality pairing, as appropriate.

Let $\mathcal{T}_h = \{K\}$ be a quasi-uniform triangulation on Ω. For $q \in \mathbb{Z}^+$, $S_h := \{v \in C^0(\Omega) \mid v|_K \in \mathcal{P}_q(K)\, \forall\, K \in \mathcal{T}_h\} \subset H^1(\Omega)$ is a piecewise polynomial subspace of C^0. We recall the classical Ritz projection operator $R_h : H^1(\Omega) \to S_h$, satisfying

$$(\nabla(R_h\varphi - \varphi), \nabla\chi) = 0 \quad \forall \chi \in S_h, \qquad (R_h\varphi - \varphi, 1) = 0. \tag{2.2}$$

The following estimates hold for Ritz projection [9]:

$$\|R_h\varphi\|_{1,p} \le C\|\varphi\|_{1,p} \qquad \forall 1 < p \le \infty, \tag{2.3}$$

$$\|\varphi - R_h\varphi\|_p + h\|\varphi - R_h\varphi\|_{1,p} \le Ch^{q+1}\|\varphi\|_{q+1,p} \qquad \forall 1 < p \le \infty. \tag{2.4}$$

The second order variable time-step scheme is based on the classical variable time-step second order BDF2 [55] and the following regularized convex-splitting uniform step size second order accurate scheme [67]: for $n \ge 1$, given $u_h^{n-1}, u_h^n \in S_h$, find $u_h^{n+1}, w_h^{n+1} \in S_h$, such that

$$\begin{cases} \left(\dfrac{3u_h^{n+1} - 4u_h^n + u_h^{n-1}}{2\tau}, v_h\right) + (\nabla w_h^{n+1}, \nabla v_h) = 0 \qquad \forall\, v_h \in S_h, \\ (w_h^{n+1}, \psi_h) = \varepsilon^2(\nabla u_h^{n+1}, \nabla\psi_h) + ((u_h^{n+1})^3 - 2u_h^n + u_h^{n-1}, \psi_h) \\ \qquad\qquad + A\tau(\nabla(u_h^{n+1} - u_h^n), \nabla\psi_h) \qquad \forall\, \psi_h \in S_h, \end{cases} \tag{2.5}$$

where u_h^n stands for the numerical solution at time t_n. Our variable time step size version of scheme (2.5) takes the following form: for $n \ge 1$, given $u_h^{n-1}, u_h^n \in S_h$, find $u_h^{n+1}, w_h^{n+1} \in S_h$, such that

$$\begin{cases} \frac{1}{\tau_{n+1}}\left(\frac{1+2\gamma_{n+1}}{1+\gamma_{n+1}}u_h^{n+1} - (1+\gamma_{n+1})\,u_h^n + \frac{(\gamma_{n+1})^2}{1+\gamma_{n+1}}u_h^{n-1}, v_h\right) = \left(\nabla w_h^{n+1}, \nabla v_h\right) \quad \forall\, v_h \in S_h, \\ \left(w_h^{n+1}, \phi_h\right) = -\left(\varepsilon^2\nabla u_h^{n+1}, \nabla\phi_h\right) + \left((1+\gamma_{n+1})\,u_h^n - \gamma_{n+1}u_h^{n-1}, \phi_h\right) \\ \qquad\qquad - \left(\left(u_h^{n+1}\right)^3, \phi_h\right) - A\tau_{n+1}\left(\nabla\left(u_h^{n+1} - u_h^n\right), \nabla\phi_h\right) \quad \forall\, \phi_h \in S_h, \end{cases} \tag{2.6}$$

where $\tau_{n+1} = t_{n+1} - t_n$ is the time-step and $\gamma_{n+1} = \frac{\tau_{n+1}}{\tau_n}$ is the ratio of the two adjacent time-steps. Moreover, we assume that $\{\gamma_n\}$ is a uniformly bounded sequence with an upper bound γ^*, i.e.,

$$\gamma_n \le \gamma^* \quad \forall n. \tag{2.7}$$

We assume that $\gamma^* \ge 1$ without loss of generality. The unique solvability of the scheme (2.6) could be easily obtained since it is the Euler–Lagrange equation for a strictly convex variational problem; see [67] for the uniform step case.

The scheme requires two initialization steps u_h^0 and u_h^1. We choose $u_h^0 = R_h u_0$ and use a standard first order convex splitting method to obtain $u_h^1, w_h^1 \in S_h$. More specifically, the initialization step is as follows: given $u_h^0 \in S_h$, find $u_h^1, w_h^1 \in S_h$, such that

$$\left\{ \begin{array}{l} \left(\dfrac{u_h^1 - u_h^0}{\tau_1}, v_h\right) + (\nabla w_h^1, \nabla v_h) = 0 \qquad \forall\, v_h \in S_h, \\ (w_h^1, \psi_h) = \varepsilon^2 (\nabla u_h^1, \nabla \psi_h) + ((u_h^1)^3 - u_h^0, \psi_h) \qquad \forall\, \psi_h \in S_h. \end{array} \right. \tag{2.8}$$

3. Energy stability and a uniform-in-time $\boldsymbol{H^1}$ stability. To facilitate the analysis below, we define the discrete Laplacian operator and the discrete H^{-1} norm. We will make use of the notation $L_0^2(\Omega) := \left\{u \in L^2(\Omega) \mid \ (u,1) = 0\right\}$, and more generally, $\mathring{V} := L_0^2 \cap V$ for any space $V \subseteq L^2(\Omega)$.

Definition 3.1. *The discrete Laplacian operator $\Delta_h : S_h \to \mathring{S}_h$ is defined as follows: for any $v_h \in S_h$, $\Delta_h v_h \in \mathring{S}_h$ denotes the unique solution to the problem*

$$(\Delta_h v_h, \chi) = -(\nabla v_h, \nabla \chi) \qquad \forall\, \chi \in S_h.$$

It is straightforward to show that by restricting the domain, $\Delta_h : \mathring{S}_h \to \mathring{S}_h$ is invertible, and for any $v_h \in \mathring{S}_h$, we have

$$(\nabla(-\Delta_h)^{-1} v_h, \nabla \chi) = (v_h, \chi) \quad \forall\, \chi \in S_h.$$

We also introduce discrete H^{-1} norm.

Definition 3.2. *The discrete H^{-1} norm, $\|\cdot\|_{-1,h}$, is defined as follows:*

$$\|v_h\|_{-1,h} := \sqrt{(v_h, (-\Delta_h)^{-1} v_h)} \quad \forall v_h \in \mathring{S}_h.$$

The following generalized Hölder inequality holds: for any $v_h \in \mathring{S}_h$,

$$\|v_h\|^2 \le \|\nabla v_h\| \|v_h\|_{-1,h}. \tag{3.1}$$

It is known that the discrete Laplacian operator defined above on the Ritz projection enjoys the following stability property [67]: let $u \in H_N^2(\Omega) := \{u \in H^2(\Omega) \mid \partial_n u = 0 \text{ on } \partial\Omega\}$; then

$$\|\Delta_h (R_h u)\| \le \|\Delta u\|\,. \tag{3.2}$$

In order to present energy stability in a numerical sense, we introduce the following discrete modified energy.

Definition 3.3. *For $n \ge 1$, the discrete energy is defined as follows:*

$$\mathcal{E}\left(u_h^{n+1}, u_h^n, \tau_{n+1}\right) = E\left(u_h^{n+1}\right) + \frac{\gamma^*}{2\left(1+\gamma^*\right)} \tau_{n+1} \left\| \frac{u_h^{n+1} - u_h^n}{\tau_{n+1}} \right\|_{-1,h}^2 + \frac{\gamma^*}{2} \|u_h^{n+1} - u_h^n\|^2,$$

where

$$E\left(u_h^{n+1}\right) = \frac{1}{4} \|u_h^{n+1}\|_{L^4}^4 - \frac{1}{2} \|u_h^{n+1}\|^2 + \frac{\varepsilon^2}{2} \|\nabla u_h^{n+1}\|^2$$

is the original energy of the discrete solution.

The following energy stability estimate is available.

THEOREM 3.1. *There exists an A_0, such that for any $A \geq A_0$, the numerical scheme* (2.6) *enjoys the following energy-decay property:*

$$\mathcal{E}\left(u_h^{n+1}, u_h^n, \tau_{n+1}\right) + (A - A_0)\tau_{n+1}\|\nabla\left(u_h^{n+1} - u_h^n\right)\|^2 \leq \mathcal{E}\left(u_h^n, u_h^{n-1}, \tau_n\right),$$

where A_0 is a constant defined by

$$A_0 = \begin{cases} 0 & \text{if } 0 < \gamma^* \leq \frac{1}{2}; \\ \frac{(1+\gamma^*)\left(\gamma^* - \frac{1}{2}\right)^2}{2(2+\gamma^*)} & \text{if } \frac{1}{2} < \gamma^* < 2; \\ \frac{(1+\gamma^*)\left(\gamma^* - \frac{1}{2}\right)^2}{2\left(2+3\gamma^* - (\gamma^*)^2\right)} & \text{if } 2 \leq \gamma^* < \frac{3}{2} + \frac{\sqrt{17}}{2}. \end{cases}$$

Proof. In (2.6), by taking $v_h = (-\Delta_h)^{-1}(u_h^{n+1} - u_h^n)$ and $\psi_h = u_h^{n+1} - u_h^n$, the two terms including w_h cancel each other out by the definition of Δ_h. Therefore,

$$\begin{aligned}
0 = {} & \frac{1}{\tau_{n+1}}\left(\frac{1+2\gamma_{n+1}}{1+\gamma_{n+1}}u_h^{n+1} - (1+\gamma_{n+1})\,u_h^n + \frac{(\gamma_{n+1})^2}{1+\gamma_{n+1}}u_h^{n-1}, (-\Delta_h)^{-1}\left(u_h^{n+1} - u_h^n\right)\right) \\
& - \left(\varepsilon^2\Delta_h u_h^{n+1}, u_h^{n+1} - u_h^n\right) - \left((1+\gamma_{n+1})\,u_h^n - \gamma_{n+1}u_h^{n-1}, u_h^{n+1} - u_h^n\right) \\
& + \left(\left(u_h^{n+1}\right)^3, u_h^{n+1} - u_h^n\right) + A\tau_{n+1}\left(\nabla\left(u_h^{n+1} - u_h^n\right), \nabla\left(u_h^{n+1} - u_h^n\right)\right) \\
:= {} & J_1 + J_2 + J_3 + J_4 + J_5.
\end{aligned}$$

For the time difference term J_1, we have

$$\begin{aligned}
J_1 = {} & \frac{1}{\tau_{n+1}}\left(\frac{1+2\gamma_{n+1}}{1+\gamma_{n+1}}u_h^{n+1} - (1+\gamma_{n+1})\,u_h^n + \frac{(\gamma_{n+1})^2}{1+\gamma_{n+1}}u_h^{n-1}, (-\Delta_h)^{-1}\left(u_h^{n+1} - u_h^n\right)\right) \\
= {} & \frac{2+4\gamma_{n+1} - (\gamma_{n+1})^2}{2\,(1+\gamma_{n+1})}\frac{\|u_h^{n+1} - u_h^n\|_{-1,h}^2}{\tau_{n+1}} - \frac{\gamma_{n+1}}{2\,(1+\gamma_{n+1})}\frac{\|u_h^n - u_h^{n-1}\|_{-1,h}^2}{\tau_n} \\
& + \frac{(\gamma_{n+1})^2}{2\,(1+\gamma_{n+1})\,\tau_{n+1}}\|u_h^{n+1} - 2u_h^n + u_h^{n-1}\|_{-1,h}^2.
\end{aligned}$$

For the highest order diffusion term J_2, we have

$$J_2 = -\left(\varepsilon^2\Delta_h u_h^{n+1}, u_h^{n+1} - u_h^n\right) = \frac{\varepsilon^2}{2}\left(\|\nabla u_h^{n+1}\|^2 - \|\nabla u_h^n\|^2 + \|\nabla u_h^{n+1} - \nabla u_h^n\|^2\right).$$

For the backwards diffusive term J_3, we have

$$\begin{aligned}
J_3 = {} & -\left((1+\gamma_{n+1})\,u_h^n - \gamma_{n+1}u_h^{n-1}, u_h^{n+1} - u_h^n\right) \\
= {} & -\left(u_h^n, u_h^{n+1} - u_h^n\right) + \gamma_{n+1}\left(u_h^{n+1} - 2u_h^n + u_h^{n-1}, u_h^{n+1} - u_h^n\right) - \gamma_{n+1}\|u_h^{n+1} - u_h^n\|^2 \\
= {} & -\frac{1}{2}\left(\|u_h^{n+1}\|^2 - \|u_h^n\|^2\right) + \left(\frac{1}{2} - \frac{\gamma_{n+1}}{2}\right)\|u_h^{n+1} - u_h^n\|^2 - \frac{\gamma_{n+1}}{2}\|u_h^n - u_h^{n-1}\|^2 \\
& + \frac{\gamma_{n+1}}{2}\|u_h^{n+1} - 2u_h^n + u_h^{n-1}\|^2.
\end{aligned}$$

For the nonlinear term J_4, we have

$$\begin{aligned}
J_4 = {} & \left(\left(u_h^{n+1}\right)^3, u_h^{n+1} - u_h^n\right) \\
= {} & \frac{1}{4}\left(\|u_h^{n+1}\|_{L^4}^4 - \|u_h^n\|_{L^4}^4\right) + \frac{1}{4}\|\left(u_h^{n+1}\right)^2 - \left(u_h^n\right)^2\|^2 + \frac{1}{2}\|u_h^{n+1}\left(u_h^{n+1} - u_h^n\right)\|^2.
\end{aligned}$$

Finally, for the stabilizing term J_5, we have

$$J_5 = A\tau_{n+1}\left(\nabla\left(u_h^{n+1}-u_h^n\right),\nabla u_h^{n+1}-u_h^n\right) = A\tau_{n+1}\|\nabla\left(u_h^{n+1}-u_h^n\right)\|^2.$$

Combining the above estimates, and ignoring some of the positive terms on the left-hand side, we have

$$\begin{aligned}
&\frac{1}{4}\|u_h^{n+1}\|_{L^4}^4 - \frac{1}{2}\|u_h^{n+1}\|^2 + \frac{\varepsilon^2}{2}\|\nabla u_h^{n+1}\|^2 + g_1(\gamma_{n+1})\frac{\|u_h^{n+1}-u_h^n\|_{-1,h}^2}{\tau_{n+1}}\\
&+\left(\frac{1}{2}-\frac{\gamma_{n+1}}{2}\right)\|u_h^{n+1}-u_h^n\|^2 + A\tau_{n+1}\|\nabla\left(u_h^{n+1}-u_h^n\right)\|^2\\
\le{}& \frac{1}{4}\|u_h^n\|_{L^4}^4 - \frac{1}{2}\|u_h^n\|^2 + \frac{\varepsilon^2}{2}\|\nabla u_h^n\|^2 + \frac{\gamma_{n+1}}{2\left(1+\gamma_{n+1}\right)}\frac{\|u_h^n-u_h^{n-1}\|_{-1,h}^2}{\tau_n} + \frac{\gamma_{n+1}}{2}\|u_h^n-u_h^{n-1}\|^2,
\end{aligned} \tag{3.3}$$

where $g_1(z) = \frac{2+4z-z^2}{2(1+z)}$. By the definition of the discrete energy $\mathcal{E}$, and the fact that γ^* is a uniform upper bound of all γ_n, the following estimate holds:

$$\begin{aligned}
&\mathcal{E}\left(u_h^{n+1},u_h^n,\tau_{n+1}\right) + \left(g_1(\gamma_{n+1}) - \frac{\gamma^*}{2\left(1+\gamma^*\right)}\right)\frac{\|u_h^{n+1}-u_h^n\|_{-1,h}^2}{\tau_{n+1}}\\
&+\left(\frac{1}{2}-\gamma^*\right)\|u_h^{n+1}-u_h^n\|^2 + A\tau_{n+1}\|\nabla\left(u_h^{n+1}-u_h^n\right)\|^2 \le \mathcal{E}\left(u_h^n,u_h^{n-1},\tau_n\right).
\end{aligned} \tag{3.4}$$

In the case $0<\gamma^*\le\frac{1}{2}$, note that $g_1(z)\ge 1$ as $0<z\le 2$. The energy-decay property naturally holds for any $A\ge 0$. In the case $\gamma^*>\frac{1}{2}$, by (3.1), for any $\alpha>0$, we have

$$\begin{aligned}
\|u_h^{n+1}-u_h^n\|^2 &= \|\nabla\left(u_h^{n+1}-u_h^n\right)\|\|u_h^{n+1}-u_h^n\|_{-1,h}\\
&\le \frac{\tau_{n+1}}{2\alpha}\|\nabla\left(u_h^{n+1}-u_h^n\right)\|^2 + \frac{\alpha\tau_{n+1}}{2}\left\|\frac{u_h^{n+1}-u_h^n}{\tau_{n+1}}\right\|_{-1,h}^2.
\end{aligned} \tag{3.5}$$

Now we need to split the case according to different ranges of γ^*. If $\frac{1}{2}<\gamma^*<2$, and setting $\alpha = \frac{2+\gamma^*}{(1+\gamma^*)(\gamma^*-\frac{1}{2})}$, then

$$g_1(\gamma_{n+1}) - \frac{\gamma^*}{2\left(1+\gamma^*\right)} - \frac{\alpha}{2}\left(\gamma^*-\frac{1}{2}\right)\ge 0. \tag{3.6}$$

The energy-decay property holds for $A\ge A_0 = \frac{(1+\gamma^*)\left(\gamma^*-\frac{1}{2}\right)^2}{2(2+\gamma^*)}$:

$$\mathcal{E}\left(u_h^{n+1},u_h^n,\tau_{n+1}\right) + \left(A-A_0\right)\tau_{n+1}\|\nabla\left(u_h^{n+1}-u_h^n\right)\|^2 \le \mathcal{E}\left(u_h^n,u_h^{n-1},\tau_n\right).$$

If $2\le\gamma^*<\frac{3+\sqrt{17}}{2}$, we set $\alpha = \frac{2+3\gamma^*-(\gamma^*)^2}{(1+\gamma^*)\left(\gamma^*-\frac{1}{2}\right)}$. It is straightforward to check that inequality (3.6) (thus the energy-decay property) still holds for $A\ge A_0 = \frac{(1+\gamma^*)\left(\gamma^*-\frac{1}{2}\right)^2}{2\left(2+3\gamma^*-(\gamma^*)^2\right)}$. ∎

Remark 3.1. In the convergence analysis, we will assume that $1\le\gamma^*<2$. As a result, a mild requirement that $A\ge 1$ is sufficient to ensure energy stability.

For the initial step, we have the following well-known stability for the initialization scheme (2.8):

$$E(u_h^1) + \tau_1\left\|\frac{u_h^1-u_h^0}{\tau_1}\right\|_{-1,h}^2 = E(u_h^1) + \tau_1\left\|\nabla w_h^1\right\|^2 \le E(u_h^0). \tag{3.7}$$

Now we are able to obtain a uniform-in-time H^1 estimate of the numerical solution similar to the constant step case (see [67]).

THEOREM 3.2. *Suppose that the initial datum is bounded in the following sense:*

$$E(u_h^0) + \frac{\gamma^*}{1+2\gamma^*}\|u_h^0\|^2 \le \frac{C_0}{1+2\gamma^*} \tag{3.8}$$

for some C_0 that is independent of h. Define $\kappa_A := A - A_0$. Then, there exists a constant C_1, which depends on C_0, Ω, γ^*, and ε but is independent of h and τ, such that for any $m \ge 1$

$$\|u_h^m\|_{H^1}^2 + \kappa_A \sum_{n=1}^{m} \tau_n \left\| \frac{u_h^n - u_h^{n-1}}{\tau_n} \right\|_{-1,h}^2 + \kappa_A \sum_{n=1}^{m} \tau_n \|w_h^n\| \le C_1. \tag{3.9}$$

4. Convergence analysis and error estimate. We denote by (u, w) the exact solution to the original Cahn–Hilliard equation (1.2). We say that the solution pair is of regularity of class $\mathcal{C}$ if and only if

$$u \in W^{3,\infty}(0,T;L^2) \cap W^{1,\infty}(0,T;H^{q+1}) \quad \text{and} \quad w \in L^\infty(0,T;H^{q+1}).$$

Such a regularity assumption on the exact solution is standard in numerical analysis.

Let us denote $u^{n+1} := u(t_{n+1}), w^{n+1} := w(t_{n+1})$; then we have

$$\begin{cases} \left(Du^{n+1}, v_h\right) = \left(\nabla w^{n+1}, \nabla v_h\right) + \left(R_1^{n+1}, v_h\right) \quad \forall v_h \in S_h, \\ \\ \left(w^{n+1}, \phi_h\right) = -\left(\varepsilon^2 \nabla u^{n+1}, \nabla \phi_h\right) + \left(T_{1,u}^n, \phi_h\right) - \left(\left(u^{n+1}\right)^3, \phi_h\right) \\ \qquad\qquad - A\tau_{n+1}\left(\nabla\left(u^{n+1} - u^n\right), \nabla\phi_h\right) \\ \qquad\qquad + \left(R_2^{n+1}, \phi_h\right) + \left(R_3^{n+1}, \phi_h\right) \quad \forall \phi_h \in S_h, \end{cases} \tag{4.1}$$

where

$$Du^{n+1} = \begin{cases} \frac{1}{\tau_{n+1}}\left(\frac{1+2\gamma_{n+1}}{1+\gamma_{n+1}}u^{n+1} - (1+\gamma_{n+1})u^n + \frac{(\gamma_{n+1})^2}{1+\gamma_{n+1}}u^{n-1}\right), & n \ge 1, \\ \frac{1}{\tau_{n+1}}\left(u^{n+1} - u^n\right), & n = 0, \end{cases}$$

$$T_{1,u}^n = (1+\gamma_{n+1})u^n - \gamma_{n+1}u^{n-1},$$

$$R_1^{n+1} = Du^{n+1} - u_t^{n+1},$$

$$R_2^{n+1} = u^{n+1} - \begin{cases} (1+\gamma_{n+1})u^n - \gamma_{n+1}u^{n-1}, & n \ge 1, \\ u^0, & n = 0, \end{cases}$$

$$R_3^{n+1} = \begin{cases} -A\tau_{n+1}\Delta\left(u^{n+1} - u^n\right), & n \ge 1, \\ 0, & n = 0. \end{cases}$$

R_1 corresponds to the truncation error associated with the variable step BDF2 time derivative, R^2 is associated with the linear extrapolation, and R_3 is determined by the discrete viscous regularization term.

It is straightforward to verify the following bounds for the truncation errors $R_1^{n+1}, R_2^{n+1}, R_3^{n+1}$.

LEMMA 4.1 (truncation errors). *If $0 < \gamma_{n+1} \le \gamma^*$, there exists a constant C, depending on γ^*, such that*

$$\|R_1^{n+1}\|^2 \le \begin{cases} C\left(\tau_{n+1} + \tau_n\right)^3 \int_{t_{n-1}}^{t_{n+1}} \|\partial_{ttt} u\|^2 \mathrm{d}s, & n \ge 1, \\ \frac{\tau_1}{3} \int_{t_0}^{t_1} \|\partial_{tt} u(s)\|^2 \mathrm{d}s, & n = 0, \end{cases} \tag{4.2}$$

$$\|R_2^{n+1}\|^2 \le \begin{cases} C\left(\tau_{n+1}+\tau_n\right)^3 \int_{t_{n-1}}^{t_{n+1}} \|\partial_{tt}u\|^2 \mathrm{d}s, & n \ge 1, \\ \tau_1 \int_{t_0}^{t_1} \|\partial_t u\|^2 \mathrm{d}s, & n = 0, \end{cases} \tag{4.3}$$

$$\|R_3^{n+1}\|^2 \le \begin{cases} A^2\left(\tau_{n+1}\right)^3 \int_{t_n}^{t_{n+1}} \|\partial_t \Delta u\,(s)\,\|^2 \mathrm{d}s, & n \ge 1, \\ 0, & n = 0. \end{cases} \tag{4.4}$$

Let us introduce the standard error functions:

$$e_u^n := u^n - u_h^n, \quad e_w^n := w^n - w_h^n, \quad \rho^{n+1} := u^{n+1} - R_h u^{n+1},$$
$$\rho_w^{n+1} := w^{n+1} - R_h w^{n+1}, \quad \sigma_h^{n+1} := R_h u^{n+1} - u_h^{n+1}.$$

Then we get $e_u^{n+1} = \rho^{n+1} + \sigma_h^{n+1}$. By definition (2.2) of Ritz projection, it holds that $(\nabla \rho_w^{n+1}, \nabla \chi) = 0$ for all $\chi \in S_h$. Together with the definition of the discrete Laplacian Δ_h, we have (see, for instance, [67])

$$(\nabla e_w^{n+1}, \nabla v_h) = (e_w^{n+1}, -\Delta_h v_h) - (w^{n+1} - R_h w^{n+1}, -\Delta_h v_h) \quad \forall v_h \in S_h. \tag{4.5}$$

Taking the difference of the scheme (2.5) and (4.1), setting $\phi_h = -\Delta_h v_h$, and adding the two equations, we deduce the following error equation:

$$\begin{aligned} &\left(D\sigma_h^{n+1}, v_h\right) + \left(\varepsilon^2 \nabla \sigma_h^{n+1}, \nabla\left(-\Delta_h v_h\right)\right) + \tau_{n+1}\left(\nabla T_2^{n+1}, \nabla(-\Delta_h v_h)\right) \\ &= \left(T_{1,\sigma}^n, -\Delta_h v_h\right) - \left(\left(u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, -\Delta_h v_h\right) + R^{n+1}(v_h), \end{aligned} \tag{4.6}$$

where

$$\begin{aligned} R^{n+1}(v_h) = &\left(R_1^{n+1}, v_h\right) + \left(R_2^{n+1}, -\Delta_h v_h\right) + \left(R_3^{n+1}, -\Delta_h v_h\right) \\ &+ \left(R_h w^{n+1} - w^{n+1}, -\Delta_h v_h\right) - \left(D\rho^{n+1}, v_h\right) + \left(T_{1,\rho}^n, -\Delta_h v_h\right), \end{aligned}$$

and

$$T_{1,\sigma}^n = \begin{cases} \left(1+\gamma_{n+1}\right)\sigma_h^n - \gamma_{n+1}\sigma_h^{n-1}, & n \ge 1, \\ 0, & n = 0, \end{cases}$$

$$T_{1,\rho}^n = \begin{cases} \left(1+\gamma_{n+1}\right)\rho^n - \gamma_{n+1}\rho^{n-1}, & n \ge 1, \\ \rho^0, & n = 0, \end{cases}$$

$$T_2^{n+1} = \begin{cases} A\left(\sigma_h^{n+1} - \sigma_h^n\right), & n \ge 1, \\ 0, & n = 0. \end{cases}$$

The following lemmas will provide estimates for all the terms on the right-hand side of the error equation.

LEMMA 4.2 (estimate for the term $R^{n+1}(v_h)$). *There exists $C > 0$ which depends on ε and γ^*, such that*

$$R^{n+1}(v_h) \le C\mathcal{R}_1^{n+1} + \frac{1}{8}\left\|v_h\right\|^2 + \frac{\varepsilon^2}{4}\left\|\Delta_h v_h\right\|^2 \quad \forall n \ge 1, \tag{4.7}$$

$$R^1(v_h) \le C\mathcal{R}_1^1 + \frac{1}{8\tau_1}\left\|v_h\right\|^2 + \frac{1}{16}\left\|v_h\right\|^2 + \frac{\varepsilon^2}{4}\left\|\Delta_h v_h\right\|^2, \tag{4.8}$$

where

$$\mathcal{R}_1^{n+1} = \left(\tau_{n+1}+\tau_n\right)^3\left(\int_{t_{n-1}}^{t_{n+1}} \|\partial_{ttt}u\|^2 \mathrm{d}s + \int_{t_{n-1}}^{t_{n+1}} \|\partial_{tt}u\|^2 \mathrm{d}s\right)$$

$$+\tau_{n+1}^3\int_{t_n}^{t_{n+1}}\|\partial_t\Delta u\,(s)\,\|^2\mathrm{d}s+\frac{h^{2(q+1)}}{\tau_{n+1}}\int_{t_{n-1}}^{t_{n+1}}\|\partial_t u\|_{H^{q+1}}^2\mathrm{d}s$$
$$+h^{2(q+1)}\left(\|w^{n+1}\|_{H^{q+1}}^2+\|u^n\|_{H^{q+1}}^2+\|u^{n-1}\|_{H^{q+1}}^2\right),$$
$$\mathcal{R}_1^1=\tau_1^2\int_{t_0}^{t_1}\|\partial_{tt}u\,(s)\,\|^2\mathrm{d}s+\tau_1^2\int_{t_0}^{t_1}\|\partial_t\Delta u\|^2\mathrm{d}s+\frac{h^{2(q+1)}}{\tau_1}\int_{t_0}^{t_1}\|\partial_t u\|_{H^{q+1}}^2\mathrm{d}s$$
$$+h^{2(q+1)}(\|w^1\|_{H^{q+1}}^2+\|u^0\|_{H^{q+1}}^2).$$

Proof. If $n\geq 1$, by the Cauchy–Schwarz inequality, $R^{n+1}(v_h)$ could be bounded by

$$R^{n+1}(v_h)\leq 4\left(\left\|R_1^{n+1}\right\|^2+\left\|D\rho^{n+1}\right\|\right)$$
$$+\frac{4}{\varepsilon^2}\left(\left\|R_2^{n+1}\right\|^2+\left\|R_3^{n+1}\right\|^2+\left\|R_hw^{n+1}-w^{n+1}\right\|^2+\left\|T_{1,\rho}^n\right\|^2\right)$$
$$+\frac{1}{8}\left\|v_h\right\|^2+\frac{\varepsilon^2}{4}\left\|\Delta_hv_h\right\|^2. \tag{4.9}$$

For the term involving w^{n+1}, by the property of Ritz projection, we have

$$\|R_hw^{n+1}-w^{n+1}\|^2\leq Ch^{2(q+1)}\|w^{n+1}\|_{H^{q+1}}. \tag{4.10}$$

The estimates for the differential term $D\rho^{n+1}$ and the concave term $T_{1,\rho}^n$ could be obtained analogously:

$$\|D\rho^{n+1}\|^2=\|\,(I-R_h)\,Du^{n+1}\|^2\leq Ch^{2(q+1)}\|Du_h^{n+1}\|^2$$
$$\leq\frac{C}{\tau_{n+1}}h^{2(q+1)}\int_{t_{n-1}}^{t_{n+1}}\|\partial_t u\|_{H^{q+1}}^2\mathrm{d}s, \tag{4.11}$$

and

$$\left\|T_{1,\rho}^n\right\|^2=\left\|(1+\gamma_{n+1})\rho^n-\gamma_{n+1}\rho^{n-1}\right\|^2$$
$$\leq Ch^{2(q+1)}((1+\gamma^*)\|u^n\|_{H^{q+1}}^2+\gamma^*\|u^{n-1}\|_{H^{q+1}}^2)$$
$$\leq Ch^{2(q+1)}(\|u^n\|_{H^{q+1}}^2+\|u^{n-1}\|_{H^{q+1}}^2). \tag{4.12}$$

If $n=0$, by the Cauchy–Schwarz inequality, the $R^1(v_h)$ could be bounded by

$$R^1(v_h)\leq 4\tau_1\left\|R_1^1\right\|^2+4\left\|D\rho^1\right\|+\left(R_2^1,-\Delta_hv_h\right)$$
$$+\frac{4}{\varepsilon^2}\left(\left\|R_3^1\right\|^2+\left\|R_hw^1-w^1\right\|^2+\left\|T_{1,\rho}^n\right\|^2\right)$$
$$+\frac{1}{16\tau_1}\left\|v_h\right\|^2+\frac{1}{16}\left\|v_h\right\|^2+\frac{3\varepsilon^2}{16}\left\|\Delta_hv_h\right\|^2. \tag{4.13}$$

For the term $\left(R_2^1,-\Delta_hv_h\right)$, we have (see [67])

$$\left(R_2^1,-\Delta_hv_h\right)\leq\frac{\varepsilon^2}{16}\|\Delta_hv_h\|^2+\frac{4C}{\varepsilon^2}\frac{h^{2(q+1)}}{\tau_1}\int_{t_0}^{t_1}\|\partial_t u\|_{H^{q+1}}^2\mathrm{d}s+\frac{1}{16\tau_1}\|v_h\|^2+4\tau_1^2\int_{t_0}^{t_1}\|\partial_t\Delta u\|^2\mathrm{d}s.$$

Following the same process for estimating $\|D\rho^{n+1}\|^2$, we have

$$\|D\rho^1\|^2=\|\,(I-R_h)\,Du^1\|^2\leq\frac{C}{\tau_1}h^{2(q+1)}\int_{t_0}^{t_1}\|\partial_t u\|_{H^{q+1}}^2\mathrm{d}s. \tag{4.14}$$

Combining all the inequalities above, we obtain the desired estimate for $R^{n+1}(v_h)$. ∎

We now deal with the nonlinear convex term.

LEMMA 4.3 (estimate for the nonlinear term). *If we take $v_h = \sigma_h^{n+1}$ in the error equation, then there exists $C > 0$, such that*

$$\left(\left(u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, \Delta_h \sigma_h^{n+1}\right) \leq \frac{C}{\varepsilon^2} h^{2(q+1)} \|u^{n+1}\|_{H^{q+1}}^2 + \frac{C}{\varepsilon^6} \|\sigma_h^{n+1}\|^2 + \frac{\varepsilon^2}{8} \|\Delta_h \sigma_h^{n+1}\|^2.$$

And if we take $v_h = \sigma_h^{n+1} - \sigma_h^n$, then there exists $C > 0$, such that

$$\begin{aligned}\left(\left(u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, \Delta_h \left(\sigma_h^{n+1} - \sigma_h^n\right)\right) \leq{}& \frac{C}{\varepsilon^2} h^{2(q+1)} \|u^{n+1}\|_{H^{q+1}}^2 + \frac{C}{\varepsilon^6} \delta \|\sigma_h^{n+1}\|^2 \\ &+ \frac{\varepsilon^2}{8} \|\Delta_h \left(\sigma_h^{n+1} - \sigma_h^n\right)\|^2 + \frac{\varepsilon^2}{16\delta} \|\Delta_h \sigma_h^{n+1}\|^2\end{aligned}$$

for any $\delta > 0$.

Proof. First we notice that

$$\left(u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3 = \left(u^{n+1}\right)^3 - \left(R_h u^{n+1}\right)^3 + \left(R_h u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3,$$

which separates the nonlinear term into two parts.

For the first part, the regularity assumption yields

$$\begin{aligned}\|\left(u^{n+1}\right)^3 - \left(R_h u^{n+1}\right)^3\|^2 &= \|\rho^{n+1}[\left(u^{n+1}\right)^2 + u^{n+1} R_h u^{n+1} + \left(R_h u^{n+1}\right)^2]\|^2 \\ &\leq 4\|\rho^{n+1}\|^2 \|\left(u^{n+1}\right)^2 + \left(R_h u^{n+1}\right)^2\|^2 \\ &\leq 8\|\rho^{n+1}\|^2 \left(\|u^{n+1}\|_{L^4}^4 + \|R_h u^{n+1}\|_{L^4}^4\right) \\ &\leq C h^{2(q+1)} \|u^{n+1}\|_{H^{q+1}}^2. \qquad (4.15)\end{aligned}$$

If we take $v_h = \sigma_h^{n+1}$, according to (4.15) and the Cauchy–Schwarz inequality, we have

$$\begin{aligned}\left(\left(u^{n+1}\right)^3 - \left(R_h u^{n+1}\right)^3, \Delta_h \sigma_h^{n+1}\right) &\leq \|\left(u^{n+1}\right)^3 - \left(R_h u^{n+1}\right)^3\| \|\sigma_h^{n+1}\| \\ &\leq \frac{C}{\varepsilon^2} h^{2(q+1)} \|u^{n+1}\|_{H^{q+1}}^2 + \frac{\varepsilon^2}{16} \|\Delta_h \sigma_h^{n+1}\|^2. \qquad (4.16)\end{aligned}$$

Similarly, if we take $v_h = \sigma_h^{n+1} - \sigma_h^n$, we have

$$\begin{aligned}\left(\left(u^{n+1}\right)^3 - \left(R_h u^{n+1}\right)^3, \Delta_h \left(\sigma_h^{n+1} - \sigma_h^n\right)\right) &\leq \|\left(u^{n+1}\right)^3 - \left(R_h u^{n+1}\right)^3\| \|\Delta_h \left(\sigma_h^{n+1} - \sigma_h^n\right)\| \\ &\leq \frac{C}{\varepsilon^2} h^{2(q+1)} \|u^{n+1}\|_{H^{q+1}}^2 + \frac{\varepsilon^2}{16} \|\Delta_h \left(\sigma_h^{n+1} - \sigma_h^n\right)\|^2. \qquad (4.17)\end{aligned}$$

For the discussion of the second part of the nonlinear term, we define $\bar{u}_0 = \frac{1}{|\Omega|}(u_0, 1)$. Then $(R_h u^n - \bar{u}_0, 1) = (u_h^n - \bar{u}_0, 1) = 0$. In particular, for all $0 \leq n \leq N_T$, observe that $\left(\sigma_h^{n+1}, 1\right) = 0$. Applying the embedding theorem $H^1(\Omega) \hookrightarrow L^6(\Omega)$, we have

$$\begin{aligned}&\left(\left(R_h u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, \Delta_h v_h\right) \\ &= \left(\left(\left(R_h u^{n+1}\right)^2 + \left(u_h^{n+1}\right)^2 + R_h u^{n+1} u_h^{n+1}\right) \sigma_h^{n+1}, \Delta_h v_h\right) \\ &\leq \|\left(R_h u^{n+1}\right)^2 + \left(u_h^{n+1}\right)^2 + R_h u^{n+1} u_h^{n+1}\|_{L^3} \|\sigma_h^{n+1}\|_{L^6} \|\Delta_h v_h\|\end{aligned}$$

$$
\begin{aligned}
&\le 2C\left(\|R_h u^{n+1}\|_{L^6}^2 + \|u_h^{n+1}\|_{L^6}^2\right)\|\nabla\sigma_h^{n+1}\|\|\Delta_h v_h\| \\
&\le 4C\left(\|R_h u^{n+1} - \bar u_0\|_{L^6}^2 + \|u_h^{n+1} - \bar u_0\|_{L^6}^2 + 2|\Omega|^{\frac13}|\bar u_0|^2\right)\|\nabla\sigma_h^{n+1}\|\|\Delta_h v_h\| \\
&\le 4C\left(\|\nabla R_h u^{n+1}\|^2 + \|\nabla u_h^{n+1}\|^2 + 2|\Omega|^{\frac13}|\bar u_0|^2\right)\|\nabla\sigma_h^{n+1}\|\|\Delta_h v_h\|.
\end{aligned}
$$

If we take $v_h = \sigma_h^{n+1}$, according to the H^1 bound of the discrete solution u_h^n, we have

$$
\begin{aligned}
&\left(\left(R_h u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, \Delta_h\sigma_h^{n+1}\right) \\
&\le C\|\nabla\sigma_h^{n+1}\|\|\Delta_h\sigma_h^{n+1}\| \le C\|\sigma_h^{n+1}\|^{\frac12}\|\Delta_h\sigma_h^{n+1}\|^{\frac32} \le \frac{C}{\varepsilon^6}\|\sigma_h^{n+1}\|^2 + \frac{\varepsilon^2}{16}\|\Delta_h\sigma_h^{n+1}\|^2,
\end{aligned} \tag{4.18}
$$

where we have utilized Young's inequality in the last step.

If we take $v_h = \sigma_h^{n+1} - \sigma_h^n$, it follows in an analogous way that

$$
\begin{aligned}
&\left(\left(R_h u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, \Delta_h\left(\sigma_h^{n+1} - \sigma_h^n\right)\right) \\
&\le C\|\nabla\sigma_h^{n+1}\|\|\Delta_h\left(\sigma_h^{n+1} - \sigma_h^n\right)\| \\
&\le C\|\sigma_h^{n+1}\|^{\frac12}\|\Delta_h\sigma_h^{n+1}\|^{\frac12}\|\Delta_h\left(\sigma_h^{n+1} - \sigma_h^n\right)\| \\
&\le \frac{C}{\varepsilon^6}\delta\|\sigma_h^{n+1}\|^2 + \frac{\varepsilon^2}{16\delta}\|\Delta_h\sigma_h^{n+1}\|^2 + \frac{\varepsilon^2}{16}\|\Delta_h\left(\sigma_h^{n+1} - \sigma_h^n\right)\|^2.
\end{aligned} \tag{4.19}
$$

As a result, if we take $v_h = \sigma_h^{n+1}$, a combination of (4.16) and (4.18) yields

$$
\left(\left(u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, \Delta_h\sigma_h^{n+1}\right) \le \frac{C}{\varepsilon^2}h^{2(q+1)}\|u^{n+1}\|_{H^{q+1}}^2 + \frac{C}{\varepsilon^6}\|\sigma_h^{n+1}\|^2 + \frac{\varepsilon^2}{8}\|\Delta_h\sigma_h^{n+1}\|^2.
$$

If we take $v_h = \sigma_h^{n+1} - \sigma_h^n$, a combination of (4.17) and (4.19) yields

$$
\begin{aligned}
\left(\left(u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, \Delta_h\left(\sigma_h^{n+1} - \sigma_h^n\right)\right) &\le \frac{C}{\varepsilon^2}h^{2(q+1)}\|u^{n+1}\|_{H^{q+1}}^2 + \frac{C}{\varepsilon^6}\delta\|\sigma_h^{n+1}\|^2 \\
&\quad + \frac{\varepsilon^2}{8}\|\Delta_h\left(\sigma_h^{n+1} - \sigma_h^n\right)\|^2 + \frac{\varepsilon^2}{16\delta}\|\Delta_h\sigma_h^{n+1}\|^2.
\end{aligned}
$$

Therefore, the desired estimate for the nonlinear term has been established. ∎

In addition, by the Cauchy–Schwarz inequality, the concave (extrapolation) term could be bounded by

$$
\begin{aligned}
&\left(T_{1,\sigma}^n, -\Delta_h v_h\right) \\
&\le \begin{cases} \frac{4}{\varepsilon^2}\left\|T_{1,\sigma}^n\right\|^2 + \frac{\varepsilon^2}{16}\|\Delta_h v_h\|^2 \le \frac{C}{\varepsilon^2}\left(\|\sigma_h^n\|^2 + \left\|\sigma_h^{n-1}\right\|^2\right) + \frac{\varepsilon^2}{16}\|\Delta_h v_h\|^2, & n \ge 1, \\ 0, & n = 0. \end{cases}
\end{aligned} \tag{4.20}
$$

Here the constant C depends on γ^*.

Together with Lemmas 4.2 and 4.3, we could get the error bounds for the right-hand side of the error equation (4.6), as is stated in the following lemma.

LEMMA 4.4 (estimate for the right-hand side of the error equation). *There exist a constant $C > 0$ which depends on ε and γ^*, and $C_2 > 0$ which depends on γ^*, such that*

$$
\left(T_{1,\sigma}^n, -\Delta_h v_h\right) - \left(\left(u^{n+1}\right)^3 - \left(u_h^{n+1}\right)^3, -\Delta_h v_h\right) + R^{n+1}(v_h)
$$

$$\le C\mathcal{R}_2^{n+1} + \frac{C_2}{\varepsilon^6}\|\sigma_h^{n+1}\|^2 + \frac{C_2}{\varepsilon^2}\left(\|\sigma_h^n\|^2 + \|\sigma_h^{n-1}\|^2\right)$$

$$+\begin{cases} \frac{1}{8}\left\|\sigma_h^{n+1}\right\|^2 + \frac{7\varepsilon^2}{16}\left\|\Delta_h\sigma_h^{n+1}\right\|^2 & \textit{if } v_h = \sigma_h^{n+1}, \forall n \ge 1, \\ \frac{1}{8}\left\|\sigma_h^{n+1} - \sigma_h^n\right\|^2 + \frac{7\varepsilon^2}{16}\left\|\Delta_h(\sigma_h^{n+1} - \sigma_h^n)\right\|^2 + \frac{\varepsilon^2}{16\delta}\left\|\Delta_h\sigma_h^{n+1}\right\|^2 & \textit{if } v_h = \sigma_h^{n+1} - \sigma_h^n, \forall n \ge 1, \end{cases}$$

$$(T_{1,\sigma}^0, -\Delta_h v_h) - \left(\left(u^1\right)^3 - \left(u_h^1\right)^3, -\Delta_h v_h\right) + R^1(v_h)$$

$$\le C\mathcal{R}_2^1 + \frac{C_2}{\varepsilon^6}\|v_h^1\|^2 + \frac{1}{8\tau_1}\|v_h\|^2 + \frac{1}{16}\|v_h\|^2 + \frac{3\varepsilon^2}{8}\|\Delta_h v_h\|^2,$$

where

$$\begin{aligned} \mathcal{R}_2^{n+1} = {} & (\tau_{n+1} + \tau_n)^3\left(\int_{t_{n-1}}^{t_{n+1}}\|\partial_{ttt}u\|^2 \mathrm{d}s + \int_{t_{n-1}}^{t_{n+1}}\|\partial_{tt}u\|^2 \mathrm{d}s\right) \\ & + \tau_{n+1}^3\int_{t_n}^{t_{n+1}}\|\partial_t\Delta u\,(s)\,\|^2 \mathrm{d}s + \frac{h^{2(q+1)}}{\tau_{n+1}}\int_{t_{n-1}}^{t_{n+1}}\|\partial_t u\|_{H^{q+1}}^2 \mathrm{d}s \\ & + h^{2(q+1)}\left(\|w^{n+1}\|_{H^{q+1}}^2 + \|u^{n+1}\|_{H^{q+1}}^2 + \|u^n\|_{H^{q+1}}^2 + \|u^{n-1}\|_{H^{q+1}}^2\right), \\ \mathcal{R}_2^1 = {} & \tau_1^2\int_{t_0}^{t_1}\|\partial_{tt}u\,(s)\,\|^2 \mathrm{d}s + \tau_1^2\int_{t_0}^{t_1}\|\partial_t\Delta u\|^2 \mathrm{d}s + \frac{h^{2(q+1)}}{\tau_1}\int_{t_0}^{t_1}\|\partial_t u\|_{H^{q+1}}^2 \mathrm{d}s \\ & + h^{2(q+1)}(\|u^1\|_{H^{q+1}}^2 + \|w^1\|_{H^{q+1}}^2 + \|u^0\|_{H^{q+1}}^2). \end{aligned}$$

Now we focus our attention on the left-hand side of the error equation (4.6).

LEMMA 4.5 (estimate for the left-hand side of the error equation). *Denote*

$$\lambda_{n+1} = \frac{\gamma_{n+1}^2}{(1+\gamma_{n+1})^2}.$$

We have, corresponding to the case of $n = 1$ in the error equation (4.6),

$$\begin{aligned} & \left(D\sigma_h^1, v_h\right) + \left(\varepsilon^2\nabla\sigma_h^1, \nabla\left(-\Delta_h v_h\right)\right) + \tau_1\left(\nabla T_2^1, \nabla(-\Delta_h v_h)\right) \\ & = \frac{1}{2\tau_1}\left(\|\sigma_h^1\|^2 - \|\sigma_h^0\|^2 + \|\sigma_h^1 - \sigma_h^0\|^2\right) + \varepsilon^2\|\Delta_h\sigma_h^1\|^2. \end{aligned}$$

For $n \ge 1$, if we take $v_h = \sigma_h^{n+1}$, the following estimate holds for the left-hand side of the error equation:

$$\begin{aligned} & \left(D\sigma_h^{n+1}, v_h\right) + \left(\varepsilon^2\nabla\sigma_h^{n+1}, \nabla\left(-\Delta_h v_h\right)\right) + \tau_{n+1}\left(\nabla T_2^{n+1}, \nabla(-\Delta_h v_h)\right) \\ & \ge \frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left(\|\sigma_h^{n+1}\|^2 - \|\sigma_h^n\|^2 - \lambda_{n+1}\left(\|\sigma_h^{n+1}\|^2 - \|\sigma_h^{n-1}\|^2\right)\right) \\ & \quad + \frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left((1-2\lambda_{n+1})\|\sigma_h^{n+1} - \sigma_h^n\|^2 - 2\lambda_{n+1}\|\sigma_h^n - \sigma_h^{n-1}\|^2\right) \\ & \quad + \left(\frac{1}{2}A\tau_{n+1} + \varepsilon^2\right)\|\Delta_h\sigma_h^{n+1}\|^2 - \frac{1}{2}A\tau_{n+1}\|\Delta_h\sigma_h^n\|^2 + \frac{1}{2}A\tau_{n+1}\|\Delta_h(\sigma_h^{n+1} - \sigma_h^n)\|^2. \end{aligned} \tag{4.21}$$

And if we take $v_h = \sigma_h^{n+1} - \sigma_h^n$, the following estimate holds for the left-hand side of the error equation:

$$\begin{aligned} & \left(D\sigma_h^{n+1}, v_h\right) + \left(\varepsilon^2\nabla\sigma_h^{n+1}, \nabla\left(-\Delta_h v_h\right)\right) + \tau_{n+1}\left(\nabla T_2^{n+1}, \nabla(-\Delta_h v_h)\right) \\ & \ge \frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left((2-3\lambda_{n+1})\|\sigma_h^{n+1} - \sigma_h^n\|^2 - \lambda_{n+1}\|\sigma_h^n - \sigma_h^{n-1}\|^2\right) \end{aligned}$$

$$+\frac{\varepsilon^2}{2}\|\Delta_h\sigma_h^{n+1}\|^2-\frac{\varepsilon^2}{2}\|\Delta_h\sigma_h^n\|^2+\left(\frac{\varepsilon^2}{2}+A\tau_{n+1}\right)\|\Delta_h(\sigma_h^{n+1}-\sigma_h^n)\|^2 \tag{4.22}$$

for any $\delta>0$.

Proof. First, we take $v_h=\sigma_h^{n+1}$. If $n\geq 1$, according to the inequality $\|\sigma_h^{n+1}-\sigma_h^{n-1}\|^2\leq 2\|\sigma_h^{n+1}-\sigma_h^n\|^2+2\|\sigma_h^n-\sigma_h^{n-1}\|^2$, the term $(D\sigma_h^{n+1},\sigma_h^{n+1})$ could be bounded below:

$$\begin{aligned}
\left(D\sigma_h^{n+1},\sigma_h^{n+1}\right)&=\frac{1}{\tau_{n+1}}\left((1+\gamma_{n+1})\left(\sigma_h^{n+1}-\sigma_h^n\right)-\frac{(\gamma_{n+1})^2}{1+\gamma_{n+1}}\left(\sigma_h^{n+1}-\sigma_h^{n-1}\right),\sigma_h^{n+1}\right)\\
&=\frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left(\|\sigma_h^{n+1}\|^2-\|\sigma_h^n\|^2+\|\sigma_h^{n+1}-\sigma_h^n\|^2\right)\\
&\quad-\frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\lambda_{n+1}\left(\|\sigma_h^{n+1}\|^2-\|\sigma_h^{n-1}\|^2+\|\sigma_h^{n+1}-\sigma_h^{n-1}\|^2\right)\\
&\geq\frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left(\|\sigma_h^{n+1}\|^2-\|\sigma_h^n\|^2-\lambda_{n+1}\left(\|\sigma_h^{n+1}\|^2-\|\sigma_h^{n-1}\|^2\right)\right)\\
&\quad+\frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left((1-2\lambda_{n+1})\|\sigma_h^{n+1}-\sigma_h^n\|^2-2\lambda_{n+1}\|\sigma_h^n-\sigma_h^{n-1}\|^2\right).
\end{aligned}$$

If $n=0$, we have

$$\left(D\sigma_h^1,\sigma_h^1\right)=\frac{1}{\tau_1}\left(\sigma_h^1-\sigma_h^0,\sigma_h^1\right)=\frac{1}{2\tau_1}\left(\|\sigma_h^1\|^2-\|\sigma_h^0\|^2+\|\sigma_h^1-\sigma_h^0\|^2\right).$$

If we take $v_h=\sigma_h^{n+1}-\sigma_h^n$, then

$$\begin{aligned}
&\left(D\sigma_h^{n+1},\sigma_h^{n+1}-\sigma_h^n\right)\\
&\geq\frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left(\frac{2+4\gamma_{n+1}-(\gamma_{n+1})^2}{(1+\gamma_{n+1})^2}\|\sigma_h^{n+1}-\sigma_h^n\|^2-\frac{(\gamma_{n+1})^2}{(1+\gamma_{n+1})^2}\|\sigma_h^n-\sigma_h^{n-1}\|^2\right)\\
&=\frac{(1+\gamma_{n+1})}{2\tau_{n+1}}\left((2-3\lambda_{n+1})\|\sigma_h^{n+1}-\sigma_h^n\|^2-\lambda_{n+1}\|\sigma_h^n-\sigma_h^{n-1}\|^2\right).
\end{aligned}$$

For the second term, we have

$$\left(\varepsilon^2\Delta_h\sigma_h^{n+1},\Delta_h\sigma_h^{n+1}\right)=\varepsilon^2\|\Delta_h\sigma_h^{n+1}\|^2,$$

and

$$\left(\varepsilon^2\Delta_h\sigma_h^{n+1},\Delta_h\left(\sigma_h^{n+1}-\sigma_h^n\right)\right)=\frac{\varepsilon^2}{2}\left(\|\Delta_h\sigma_h^{n+1}\|^2-\|\Delta_h\sigma_h^n\|^2+\|\Delta_h(\sigma_h^{n+1}-\sigma_h^n)\|^2\right).$$

For the last term, we have

$$\left(\Delta_hT_2^{n+1},\Delta_h\sigma_h^{n+1}\right)=\begin{cases}\frac{A\tau_{n+1}}{2}\left(\|\Delta_h\sigma_h^{n+1}\|^2-\|\Delta_h\sigma_h^n\|^2+\|\Delta_h(\sigma_h^{n+1}-\sigma_h^n)\|^2\right), & n\geq 1,\\ 0, & n=0,\end{cases}$$

and

$$\left(\Delta_hT_2^{n+1},\Delta_h\left(\sigma_h^{n+1}-\sigma_h^n\right)\right)=A\tau_{n+1}\|\Delta_h(\sigma_h^{n+1}-\sigma_h^n)\|^2.$$

After summing up all these terms, we could obtain the estimate for the left-hand side of the error equation for $v_h=\sigma_h^{n+1}$ and $v_h=\sigma_h^{n+1}-\sigma_h^n$. ∎

A combination of the previous lemmas gives rise to the following estimate.

LEMMA 4.6. *Let us take $v_h = \sigma_h^{n+1} + \delta(\sigma_h^{n+1} - \sigma_h^n)$ in the error equation. If $n \geq 1$, then there exists a constant $C_3 > 0$ which depends on ε and γ^*, such that*

$$\begin{aligned}
&\|\sigma_h^{n+1}\|^2 - \|\sigma_h^n\|^2 - \lambda_{n+1}\left(\|\sigma_h^{n+1}\|^2 - \|\sigma_h^{n-1}\|^2\right)\\
&+(1+2\delta-(2+3\delta)\lambda_{n+1})\|\sigma_h^{n+1}-\sigma_h^n\|^2 - \lambda_{n+1}(\delta+2)\|\sigma_h^n - \sigma_h^{n-1}\|^2\\
&+\frac{1}{2}\left(\varepsilon^2(1+\delta)+A\tau_{n+1}\right)\mu_{n+1}\tau_{n+1}\|\Delta_h\sigma_h^{n+1}\|^2 - \frac{1}{2}(\varepsilon^2\delta + A\tau_{n+1})\mu_{n+1}\gamma_{n+1}\tau_n\|\Delta_h\sigma_h^n\|^2\\
&+\frac{1}{2}\left(\frac{\varepsilon^2}{8}\delta + A\tau_{n+1}(1+2\delta)\right)\mu_{n+1}\tau_{n+1}\|\Delta_h(\sigma_h^{n+1}-\sigma_h^n)\|^2\\
\leq\ & C_3(1+\delta)\mu_{n+1}\tau_{n+1}\left(\|\sigma_h^{n+1}\|^2 + \|\sigma_h^n\|^2 + \|\sigma_h^{n-1}\|^2\right) + C\mathcal{R}^{n+1} \quad \forall n \geq 1,
\end{aligned} \tag{4.23}$$

$$\|\sigma_h^1\|^2 + \varepsilon^2\tau_1\|\Delta_h\sigma_h^1\|^2 \leq C_3\tau_1\|\sigma_h^1\|^2 + C\mathcal{R}^1, \tag{4.24}$$

where $\mu_{n+1} = \frac{2}{1+\gamma_{n+1}}$ and

$$\begin{aligned}
\mathcal{R}^{n+1} =\ & (\tau_{n+1}+\tau_n)^3\,\tau_{n+1}\left(\int_{t_{n-1}}^{t_{n+1}}\|\partial_{ttt}u\|^2\mathrm{d}s + \int_{t_{n-1}}^{t_{n+1}}\|\partial_{tt}u\|^2\mathrm{d}s\right)\\
&+\tau_{n+1}^4\int_{t_n}^{t_{n+1}}\|\partial_t\Delta u\,(s)\,\|^2\mathrm{d}s + h^{2(q+1)}\int_{t_{n-1}}^{t_{n+1}}\|\partial_t u\|_{H^{q+1}}^2\mathrm{d}s\\
&+h^{2(q+1)}\tau_{n+1}\left(\|w^{n+1}\|_{H^{q+1}}^2 + \|u^n\|_{H^{q+1}}^2 + \|u^{n-1}\|_{H^{q+1}}^2 + \|u^{n+1}\|_{H^{q+1}}^2\right),\\
\mathcal{R}^1 =\ & \tau_1^3\int_{t_0}^{t_1}\|\partial_{tt}u\,(s)\,\|^2\mathrm{d}s + \tau_1^3\int_{t_0}^{t_1}\|\partial_t\Delta u\|^2\mathrm{d}s\\
&+h^{2(q+1)}\left(\int_{t_0}^{t_1}\|\partial_t u\|_{H^{q+1}}^2\mathrm{d}s + \tau_1\left(\|w^1\|_{H^{q+1}}^2 + \|u^0\|_{H^{q+1}}^2 + \|u^1\|_{H^{q+1}}^2\right)\right).
\end{aligned}$$

Following the idea of Becker [7], a crude L^2 error estimate for u_h with an exponential growth factor could be obtained in a straightforward manner. We leave the details to the interested reader.

THEOREM 4.7. *For any given final time $T = \sum_{n=0}^{N_T}\tau_{n+1} > 0$, assume that the exact solution pair (u, w) is in the regularity class $\mathcal{C}$, and define*

$$\Gamma_n = \sum_{k=3}^{n}[\gamma_{k-1} - \gamma_{k+1}]_+. \tag{4.25}$$

If the maximum time step size τ satisfies

$$\tau = \max_{0\leq n\leq N_T}\tau_{n+1} < \frac{1}{40C_3\,(1+\delta)},$$

then there exists $\gamma_B^* \in (1, 2)$, such that if $\gamma_n \leq \gamma_B^*$, we have the following error estimate:

$$\|e_u^{n+1}\|^2 = \|u^{n+1} - u_h^{n+1}\|^2 \leq C\left(T, \varepsilon, \gamma^*, E(u_h^0), \Gamma_n\right)\mathcal{R},$$

where $\mathcal{R}$ is as defined in (1.6), and $C\left(T, \varepsilon, \gamma^*, E(u_h^0), \Gamma_n\right)$ may depend on $T, \varepsilon, \gamma^*, E(u_h^0)$, and $\exp(C\Gamma_n)$.

Remark 4.1. The exponential prefactor $\exp(C\Gamma_n)$ appears in all existing work, even in the linear case [7, 55]. This prefactor could blow up for certain time-step series at vanishing time-steps. A specific example is the following. Fix a constant $\varsigma > 1$; for a choice of the initial step size τ_1, the first four items of the time-step series are set to be $\tau_1, \varsigma\tau_1, \varsigma\tau_1, \tau_1$. The rest of this time series τ_n is obtained by repeating the first four items for $\frac{N_T}{4}$ times. Therefore, for $T = \frac{N_T}{2}(\varsigma+1)\tau_1$,

$$\Gamma_{N_T} = \sum_{n=3}^{N_T}[\gamma_{n-1} - \gamma_{n+1}]_+ = N_T\left(\varsigma - \frac{1}{\varsigma}\right) \to \infty$$

when τ_1 tends to zero. Even for a moderate value of Γ_{N_T}, $\exp(C\Gamma_{N_T})$ could be huge—effectively infinity—due to the nature of the exponential function.

5. Optimal convergence analysis. In this section, we derive a second order in time error estimate without the undesirable exponential factor $\exp(C\Gamma_n)$. A common tool for error estimates for the evolution equation is the discrete Gronwall inequality. Unfortunately, the classical discrete Gronwall inequality such as that presented in [55] is not directly applicable to the error inequality (4.23) since it involves the difference of positive terms. A key ingredient in overcoming this difficulty is the following novel technical lemma. It can be viewed as a new generalized discrete Gronwall inequality that is able to deal with the current situation.

LEMMA 5.1 (generalized discrete Gronwall inequality). *Assume that $a_n, b_n, c_n, \theta_n, \tau_n, \mathcal{R}^n$, and ν_n are nonnegative sequences satisfying $\frac{\tau_{n+1}}{\tau_n} \le \gamma^*$ and $0 < \nu_n \le \bar\nu < 1$. If there exists a constant $0 < \eta \le 1$ such that*

$$\begin{aligned}a_{n+1} - a_n + b_{n+1} + \theta_{n+1}\tau_{n+1}c_{n+1} \le \nu_{n+1}(a_n - a_{n-1} + b_n + \theta_n\tau_n c_n) + \eta(1-\bar\nu)\theta_n\tau_n c_n \\ +C_4\tau_{n+1}(a_{n+1} + a_n + a_{n-1}) + \mathcal{R}^{n+1} \quad \forall n \ge 1,\end{aligned}$$

then

$$\begin{aligned}&a_{n+1} + \sum_{m=1}^{n} b_{m+1} + \theta_{n+1}\tau_{n+1}c_{n+1} + (1-\eta)\sum_{m=1}^{n-1}\theta_{m+1}\tau_{m+1}c_{m+1} \\ &\le \frac{C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar\nu}\sum_{k=1}^{n+1}\tau_k a_k + \mathcal{R}'_n,\end{aligned} \tag{5.1}$$

where

$$\mathcal{R}'_n = \left(\frac{C_4}{1-\bar\nu}\tau_2 + \frac{\bar\nu}{1-\bar\nu}\right)a_0 + \frac{1}{1-\bar\nu}a_1 + \left(\eta + \frac{\bar\nu}{1-\bar\nu}\right)\theta_1\tau_1c_1 + \frac{\bar\nu}{1-\bar\nu}b_1 + \frac{1}{1-\bar\nu}\sum_{k=1}^{n}\mathcal{R}^{k+1}.$$

Moreover, if we have the time-step restriction $\tau_{n+1} < \frac{1-\bar\nu}{2C_4(1+\gamma^*+(\gamma^*)^2)}$, we then have

$$a_{n+1} \le 2\exp\left(\frac{2C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar\nu}\sum_{k=1}^{n}\tau_k\right)\mathcal{R}'_n.$$

Proof. The following inequality follows from recursion and can be verified via induction:

$$a_{m+1} - a_m + b_{m+1} + \theta_{m+1}\tau_{m+1}c_{m+1}$$

$$\le \prod_{j=2}^{m+1}\nu_j(a_1-a_0+b_1+\theta_1\tau_1c_1)+\eta(1-\bar\nu)\sum_{k=1}^{m}\prod_{j=k+2}^{m+1}\nu_j\theta_k\tau_kc_k$$
$$+C_4\sum_{k=1}^{m}\prod_{j=k+2}^{m+1}\nu_j\tau_{k+1}(a_{k+1}+a_k+a_{k-1})+\sum_{k=1}^{m}\prod_{j=k+2}^{m+1}\nu_j\mathcal{R}^{k+1}.$$

Here we have adopted the convention that a product with empty indices is one.

Since $0<\nu_{n+1}\le\bar\nu<1$, $\prod_{j=2}^{m+1}\nu_j\le\bar\nu^m$ and $\prod_{j=k+2}^{m+1}\nu_j\le\bar\nu^{m-k}$. Hence

$$a_{m+1}-a_m+b_{m+1}+\theta_{m+1}\tau_{m+1}c_{m+1}$$
$$\le\bar\nu^m|a_1-a_0+b_1+\theta_1\tau_1c_1|+\eta(1-\bar\nu)\sum_{k=1}^{m}\bar\nu^{m-k}\theta_k\tau_kc_k$$
$$+C_4\sum_{k=1}^{m}\bar\nu^{m-k}\tau_{k+1}(a_{k+1}+a_k+a_{k-1})+\sum_{k=1}^{m}\bar\nu^{m-k}\mathcal{R}^{k+1}.$$

Summing up m from 1 to n and exchanging summation orders, we have

$$a_{n+1}-a_1+\sum_{m=1}^{n}b_{m+1}+\sum_{m=1}^{n}\theta_{m+1}\tau_{m+1}c_{m+1}$$
$$\le|a_1-a_0+b_1+\theta_1\tau_1c_1|\sum_{m=1}^{n}\bar\nu^m+\eta(1-\bar\nu)\sum_{m=1}^{n}\sum_{k=1}^{m}\bar\nu^{m-k}\theta_k\tau_kc_k$$
$$+C_4\sum_{m=1}^{n}\sum_{k=1}^{m}\bar\nu^{m-k}\tau_{k+1}(a_{k+1}+a_k+a_{k-1})+\sum_{m=1}^{n}\sum_{k=1}^{m}\bar\nu^{m-k}\mathcal{R}^{k+1}$$
$$=|a_1-a_0+b_1+\theta_1\tau_1c_1|\sum_{k=1}^{n}\bar\nu^m+\eta(1-\bar\nu)\sum_{k=1}^{n}\theta_k\tau_kc_k\left(\sum_{m=k}^{n}\bar\nu^{m-k}\right)$$
$$+C_4\sum_{k=1}^{n}\tau_{k+1}(a_{k+1}+a_k+a_{k-1})\left(\sum_{m=k}^{n}\bar\nu^{m-k}\right)+\sum_{k=1}^{n}\mathcal{R}^{k+1}\left(\sum_{m=k}^{n}\bar\nu^{m-k}\right).$$

Since $\frac{\tau_{n+1}}{\tau_n}\le\gamma^*$, we have

$$a_{n+1}-a_1+\sum_{m=1}^{n}b_{m+1}+\sum_{m=1}^{n}\theta_{m+1}\tau_{m+1}c_{m+1}$$
$$\le\frac{\bar\nu}{1-\bar\nu}(a_0+a_1+b_1+\theta_1\tau_1c_1)+\eta\sum_{k=1}^{n}\theta_k\tau_kc_k+\frac{C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar\nu}\sum_{k=1}^{n+1}\tau_ka_k+\frac{C_4}{1-\bar\nu}\tau_2a_0$$
$$+\frac{1}{1-\bar\nu}\sum_{k=1}^{n}\mathcal{R}^{k+1}.$$

After moving $\eta\sum_{k=1}^{n-1}\theta_{k+1}\tau_{k+1}c_{k+1}$ to the left side of the inequality, moving a_1 to the right side of the inequality, and absorbing the miscellaneous terms into R'_n, we obtain (5.1):

$$a_{n+1}+\sum_{m=1}^{n}b_{m+1}+\theta_{n+1}\tau_{n+1}c_{n+1}+(1-\eta)\sum_{m=1}^{n-1}\theta_{m+1}\tau_{m+1}c_{m+1}$$

$$\leq \frac{C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar{\nu}} \sum_{k=1}^{n+1} \tau_k a_k + \mathcal{R}'_n.$$

Moving $\frac{C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar{\nu}}\tau_{n+1}a_{n+1}$ to the left of the inequality, and utilizing the additional time-step constraint on τ_{n+1} which makes $1-\frac{C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar{\nu}}\tau_{n+1}$ larger than $\frac{1}{2}$, we obtain, after multiplying by 2,

$$\begin{aligned}&a_{n+1} + 2\sum_{m=1}^{n} b_{m+1} + 2\theta_{n+1}\tau_{n+1}c_{n+1} + 2(1-\eta)\sum_{m=1}^{n-1}\theta_{m+1}\tau_{m+1}c_{m+1}\\ &\leq \frac{2C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar{\nu}} \sum_{k=1}^{n} \tau_k a_k + 2\mathcal{R}'_n.\end{aligned}$$

The classical discrete Gronwall's inequality [55] then yields

$$\begin{aligned}&a_{n+1} + 2\sum_{m=1}^{n} b_{m+1} + 2\theta_{n+1}\tau_{n+1}c_{n+1} + 2(1-\eta)\sum_{m=1}^{n-1}\theta_{m+1}\tau_{m+1}c_{m+1}\\ &\leq 2\exp\left(\frac{2C_4(1+\gamma^*+(\gamma^*)^2)}{1-\bar{\nu}} \sum_{k=1}^{n} \tau_k\right)\mathcal{R}'_n.\end{aligned}$$

This ends the proof of the lemma. ∎

Our plan now is to recast the error inequality (4.23) into the form of (5.1) so that the novel generalized discrete Gronwall inequality is applicable.

For this purpose, we recall the following simple useful facts. They will be utilized in our final theorem, Theorem 5.2: For $0<\zeta<1$, let us define

$$\ell(\zeta) = \frac{2\sqrt{13}}{3}\cos\left(\frac{1}{3}\arccos\left(-\frac{27\zeta}{26\sqrt{13}} - \frac{8}{13\sqrt{13}}\right)\right) - \frac{2}{3}. \tag{5.2}$$

It is easy to check that $\ell(\zeta)$ is one of the roots of the equation

$$x^3 + 2x^2 - 3x - (2-\zeta) = 0, \tag{5.3}$$

and the other two roots of the equation (5.3) are less than zero. Thus we can conclude that for all $0<z<\ell(\zeta)$, we have

$$z^3 + 2z^2 - 3z - (2-\zeta) < 0. \tag{5.4}$$

Moreover, the function $\ell(\zeta)$ monotonically decreases in ζ. So we have

$$\ell(\zeta) < \ell(0) = \frac{2\sqrt{13}}{3}\cos\left(\frac{1}{3}\arccos\left(-\frac{8}{13\sqrt{13}}\right)\right) - \frac{2}{3} \approx 1.343 < 1+\sqrt{2}.$$

Now we turn to establishing the optimal convergence result.

THEOREM 5.2. *For any given final time $T=\sum_{n=0}^{N_T}\tau_{n+1}>0$ and $0<\zeta<1$, suppose that the exact solution pair (u,w) is in the regularity class $\mathcal{C}$. Assume $1\leq \gamma^*\leq \ell(\zeta)$, and the time step size is bounded by*

$$0<\tau=\max_{0\leq n\leq N_T}\tau_{n+1} < \min\left\{\frac{\varepsilon^2\zeta}{2A\gamma^*}, \frac{(1+2\gamma^*-(\gamma^*)^2)^2}{8C_3(1+2\gamma^*)(1+\gamma^*+(\gamma^*)^2)(1+\gamma^*)^2}\right\}. \tag{5.5}$$

Then, the following error estimate holds:

$$\|e_u^{n+1}\|^2 = \|u^{n+1} - u_h^{n+1}\|^2 \le C\mathcal{R}, \tag{5.6}$$

where $\mathcal{R}$ *is as defined in* (1.6)*, and* $C = C(T, \varepsilon, \gamma^*, \zeta, E(u_h^0))$ *may depend on* $T, \varepsilon, \gamma^*, \zeta$, *and initial energy* $E(u_h^0)$.

Proof. In order to apply our generalized discrete Gronwall inequality (Lemma 5.1), we recall and introduce some notation:

$$\gamma_{n+1} = \frac{\tau_{n+1}}{\tau_n}, \quad \mu_{n+1} = \frac{2}{1+\gamma_{n+1}}, \quad \lambda_{n+1} = \frac{\gamma_{n+1}^2}{(1+\gamma_{n+1})^2}.$$

It is easy to see, from the definition of $\ell(\zeta)$, that

$$\gamma^{n+1} \le \gamma^* < \ell(0) < 1 + \sqrt{2}.$$

Hence, for all $1 \le n \le N_T$,

$$0 < \frac{\lambda_{n+1}}{1-\lambda_{n+1}} = \frac{(\gamma_{n+1})^2}{1+2\gamma_{n+1}} \le \frac{(\gamma^*)^2}{1+2\gamma^*} < 1. \tag{5.7}$$

Now, for a fixed γ^*, we define $\delta = \delta^* \triangleq \frac{(1+\gamma^*)^2}{1+2\gamma^*-(\gamma^*)^2} > 0$. This implies

$$\left(\frac{1}{\lambda_{n+1}}(1+2\delta^*) - 2 - 3\delta^*\right)\frac{\lambda_{n+1}}{1-\lambda_{n+1}} \ge \delta^* + 2, \tag{5.8}$$

since $\lambda_{n+1} \le (\frac{\gamma^*}{1+\gamma^*})^2$ and

$$\begin{aligned}&\left(\frac{1}{\lambda_{n+1}}(1+2\delta^*) - 2 - 3\delta^*\right)\frac{\lambda_{n+1}}{1-\lambda_{n+1}} - (\delta^*+2)\\ &= \frac{1}{1-\lambda_{n+1}}\left((1-2\lambda_{n+1})\delta^* - 1\right) \ge \frac{1}{1-\lambda_{n+1}}\left(\left(1 - 2\left(\frac{\gamma^*}{1+\gamma^*}\right)^2\right)\delta^* - 1\right) = 0.\end{aligned}$$

Now for $0 < \tau_{n+1} \le \frac{\varepsilon^2}{2A\gamma^*}\zeta$, and $\gamma_{n+1} < 2$, we have

$$\frac{\delta^* + \frac{A}{\varepsilon^2}\tau_{n+1}}{1+\delta^* + \frac{A}{\varepsilon^2}\tau'}\gamma_{n+1} < \frac{\delta^*}{1+\delta^*}\gamma_{n+1} + \frac{\zeta}{1+\delta^*}, \tag{5.9}$$

where $\tau' = \tau_n$ or τ_{n+1}.

Let us introduce the following auxiliary variables corresponding to the variables in our generalized discrete Gronwall inequality:

$$\theta_{n+1} = \frac{1}{2}\left(\varepsilon^2(1+\delta^*) + A\tau_{n+1}\right)\frac{\mu_{n+1}}{1-\lambda_{n+1}}, \quad \xi_{n+1} = \frac{\delta^* + \frac{A}{\varepsilon^2}\tau_{n+1}}{1+\delta^* + \frac{A}{\varepsilon^2}\tau_{n+1}}\gamma_{n+1},$$
$$\text{and} \quad \nu_{n+1} = \frac{\lambda_{n+1}}{1-\lambda_{n+1}}.$$

We then deduce, after utilizing (5.7),

$$0 < \nu_{n+1} \le \bar{\nu} \triangleq \frac{(\gamma^*)^2}{1+2\gamma^*} < 1, \tag{5.10}$$

and by (5.9),

$$\xi_{n+1} < 1, \tag{5.11}$$

since $\gamma_{n+1} \le \gamma^* \le \ell(\zeta)$, and by (5.4), we have

$$\xi_{n+1} - 1 < \frac{\delta^*}{1+\delta^*}\gamma^* + \frac{\zeta}{1+\delta^*} - 1 = \frac{(\gamma^*)^3 + 2(\gamma^*)^2 - 3\gamma^* - (2-\zeta)}{1+\delta^*} \le 0.$$

Here we remark that the choice of ζ and $\gamma^* \le \ell(\zeta)$ stems from the constraint (5.11).

We claim that the following important inequality holds:

$$0 < \xi_{n+1}\frac{\theta_{n+1}}{\theta_n} - \nu_{n+1} < \left(1 - \frac{(\gamma^*)^2}{1+2\gamma^*}\right)\eta = (1-\bar{\nu})\eta, \tag{5.12}$$

where $\eta = \frac{(\gamma^*)^3+\gamma^*}{2(1+2\gamma^*-(\gamma^*)^2)} + \frac{\zeta}{4}$.

Here we first check that $0 < \eta \le 1$ before we prove (5.12). Since $0 < \gamma^{n+1} \le \gamma^* \le \ell(\zeta)$, $(\gamma^*)^3 + 2(\gamma^*)^2 - 3\gamma^* - 2 \le -\zeta$ and $0 < 1 + 2\gamma^* - (\gamma^*)^2 \le 2$. Hence, we have

$$\eta - 1 = \frac{1}{2(1+2\gamma^* - (\gamma^*)^2)}\left((\gamma^*)^3 + 2(\gamma^*)^2 - 3\gamma^* - 2 + \frac{\zeta}{2}(1 + 2\gamma^* - (\gamma^*)^2)\right) \le 0.$$

Next, we consider the term

$$\xi_{n+1}\frac{\theta_{n+1}}{\theta_n} - \nu_{n+1} = \frac{(\delta^* + \frac{A}{\varepsilon^2}\tau_{n+1})\gamma_{n+1}}{1+\delta^* + \frac{A}{\varepsilon^2}\tau_n}\frac{1+\gamma_{n+1}}{1+2\gamma_{n+1}}\frac{1+2\gamma_n}{1+\gamma_n} - \frac{\gamma_{n+1}^2}{1+2\gamma_{n+1}}.$$

First, we notice that $\frac{A}{\varepsilon^2}\tau_n \le \frac{\zeta}{2\gamma^*} < \frac{1}{2}$. Therefore,

$$\frac{\delta^* + \frac{A}{\varepsilon^2}\tau_{n+1}}{1+\delta^* + \frac{A}{\varepsilon^2}\tau_n}\frac{1+2\gamma_n}{1+\gamma_n} - \frac{\gamma^{n+1}}{1+\gamma_{n+1}} > \frac{\delta^*}{2+\delta^*} - \frac{\gamma*}{1+\gamma^*} = \frac{2(\gamma^*)^3 - 3(\gamma^*)^2 + 1}{(3+6\gamma^* - (\gamma^*)^2)(1+\gamma^*)} \ge 0.$$

Henceforth, we obtain the lower bound of (5.12):

$$\xi_{n+1}\frac{\theta_{n+1}}{\theta_n} - \nu_{n+1} = \frac{\gamma_{n+1}(1+\gamma_{n+1})}{1+2\gamma_{n+1}}\left(\frac{\delta^* + \frac{A}{\varepsilon^2}\tau_{n+1}}{1+\delta^* + \frac{A}{\varepsilon^2}\tau_n}\frac{1+2\gamma_n}{1+\gamma_n} - \frac{\gamma_{n+1}}{1+\gamma_{n+1}}\right) > 0.$$

As for the upper bound, we utilize (5.9) and $0 < \gamma_n \le \gamma^*$ to deduce

$$\begin{aligned}
\xi_{n+1}\frac{\theta_{n+1}}{\theta_n} - \nu_{n+1} &\le \frac{1+2\gamma^*}{1+\gamma^*}\frac{(\delta^* + \frac{A}{\varepsilon^2}\tau_{n+1})\gamma_{n+1}}{1+\delta^* + \frac{A}{\varepsilon^2}\tau_n}\frac{1+\gamma_{n+1}}{1+2\gamma_{n+1}} - \frac{\gamma_{n+1}^2}{1+2\gamma_{n+1}} \\
&\le \frac{1+2\gamma^*}{1+\gamma^*}\left(\frac{\delta^*\gamma_{n+1}}{1+\delta^*} + \frac{\zeta}{2(1+\delta^*)}\right)\frac{1+\gamma_{n+1}}{1+2\gamma_{n+1}} - \frac{\gamma_{n+1}^2}{1+2\gamma_{n+1}} \\
&\le \frac{\delta^*\gamma^*}{1+\delta^*} + \frac{\zeta}{2(1+\delta^*)} - \frac{(\gamma^*)^2}{1+2\gamma^*},
\end{aligned} \tag{5.13}$$

where, in the third inequality, we utlized the monotonicity of $\frac{1+2\gamma^*}{1+\gamma^*}(\frac{\delta^* x}{1+\delta^*} + \frac{\zeta}{2(1+\delta^*)})\frac{1+x}{1+2x} - \frac{x^2}{1+2x}$, which itself follows from the monotonicity of $\frac{x^2}{1+2x}$ and $-\frac{1}{2(1+2x)}$, $-\zeta(1+2\gamma^* - (\gamma^*)^2) + 2(1+\gamma^*)^2 > 0$ for $\zeta < 1$, and

$$\frac{1+2\gamma^*}{1+\gamma^*}\left(\frac{\delta^* x}{1+\delta^*} + \frac{\zeta}{2(1+\delta^*)}\right)\frac{1+x}{1+2x} - \frac{x^2}{1+2x}$$

$$= \left(\frac{1+\gamma^*}{2} - 1\right)\frac{x^2}{1+2x} - \frac{-\zeta(1+2\gamma^*-(\gamma^*)^2)+2(1+\gamma^*)^2}{4(1+\gamma^*)}\frac{1}{2(1+2x)}$$
$$+ \frac{\zeta(1+2\gamma^*-(\gamma^*)^2)+2(1+\gamma^*)^2}{8(1+\gamma^*)}.$$

After substituting δ^* into the upper bound (5.13), we obtain the upper bound of (5.12):

$$\xi_{n+1}\frac{\theta_{n+1}}{\theta_n} - \nu_{n+1} \le \frac{(\gamma^*)^3+\gamma^*}{2(1+2\gamma^*)} + \frac{\zeta(1+2\gamma^*-(\gamma^*)^2)}{4(1+2\gamma^*)} = \left(1 - \frac{(\gamma^*)^2}{1+2\gamma^*}\right)\eta.$$

We are now in the position to prove our main theorem. Following Lemma 4.6, after throwing away the term $\|\Delta_h(\sigma_h^{n+1}-\sigma_h^n)\|^2$ and multiplying $\frac{1}{1-\lambda_{n+1}} > 0$ by both sides of the inequality (4.23), we have

$$\begin{aligned}
&\|\sigma_h^{n+1}\|^2 - \|\sigma_h^n\|^2 + \left(\frac{1}{\lambda_{n+1}}(1+2\delta) - 2 - 3\delta\right)\frac{\lambda_{n+1}}{1-\lambda_{n+1}}\|\sigma_h^{n+1}-\sigma_h^n\|^2\\
&+\frac{1}{2}\left(\varepsilon^2(1+\delta)+A\tau_{n+1}\right)\frac{\mu_{n+1}}{1-\lambda_{n+1}}\tau_{n+1}\|\Delta_h\sigma_h^{n+1}\|^2\\
\le& \frac{\lambda_{n+1}}{1-\lambda_{n+1}}\left(\|\sigma_h^n\|^2 - \|\sigma_h^{n-1}\|^2 + (\delta+2)\|\sigma_h^n - \sigma_h^{n-1}\|^2\right)\\
&+\frac{1}{2}(\varepsilon^2\delta + A\tau_{n+1})\frac{\mu_{n+1}}{1-\lambda_{n+1}}\gamma_{n+1}\tau_n\|\Delta_h\sigma_h^n\|^2\\
&+C_3(1+\delta)\frac{\mu_{n+1}}{1-\lambda_{n+1}}\tau_{n+1}\left(\|\sigma_h^{n+1}\|^2 + \|\sigma_h^n\|^2 + \|\sigma_h^{n-1}\|^2\right) + \frac{C}{1-\lambda_{n+1}}\mathcal{R}^{n+1}.
\end{aligned} \tag{5.14}$$

Substituting (5.8) into (5.14), we deduce

$$\begin{aligned}
&\|\sigma_h^{n+1}\|^2 - \|\sigma_h^n\|^2 + (\delta^*+2)\|\sigma_h^{n+1}-\sigma_h^n\|^2 + \theta_{n+1}\tau_{n+1}\|\Delta_h\sigma_h^{n+1}\|^2\\
\le& \nu_{n+1}\left(\|\sigma_h^n\|^2 - \|\sigma_h^{n-1}\|^2 + (\delta^*+2)\|\sigma_h^n-\sigma_h^{n-1}\|^2\right) + \xi_{n+1}\theta_{n+1}\tau_n\|\Delta_h\sigma_h^n\|^2\\
&+C_3(1+\delta^*)\frac{\mu_{n+1}}{1-\lambda_{n+1}}\tau_{n+1}\left(\|\sigma_h^{n+1}\|^2 + \|\sigma_h^n\|^2 + \|\sigma_h^{n-1}\|^2\right) + \frac{C}{1-\lambda_{n+1}}\mathcal{R}^{n+1}.
\end{aligned} \tag{5.15}$$

Since $0 < \mu_{n+1} < 2$, $\frac{1}{1-\lambda_{n+1}} \le \frac{(1+\gamma^*)^2}{1+2\gamma^*} = 1+\bar{\nu}$, and $\theta_n > 0$, and by (5.12), we obtain

$$\begin{aligned}
&\|\sigma_h^{n+1}\|^2 - \|\sigma_h^n\|^2 + (\delta^*+2)\|\sigma_h^{n+1}-\sigma_h^n\|^2 + \theta_{n+1}\tau_{n+1}\|\Delta_h\sigma_h^{n+1}\|^2\\
\le&\nu_{n+1}\left(\|\sigma_h^n\|^2 - \|\sigma_h^{n-1}\|^2 + (\delta^*+2)\|\sigma_h^n-\sigma_h^{n-1}\|^2 + \theta_n\tau_n\|\Delta_h\sigma_h^n\|^2\right)\\
&+\left(\xi_{n+1}\frac{\theta_{n+1}}{\theta_n} - \nu_{n+1}\right)\theta_n\tau_n\|\Delta_h\sigma_h^n\|^2 + 2C_3(1+\delta^*)\tau_{n+1}\left(\|\sigma_h^{n+1}\|^2 + \|\sigma_h^n\|^2 + \|\sigma_h^{n-1}\|^2\right) + C\mathcal{R}^{n+1}\\
\le&\nu_{n+1}\left(\|\sigma_h^n\|^2 - \|\sigma_h^{n-1}\|^2 + (\delta^*+2)\|\sigma_h^n-\sigma_h^{n-1}\|^2 + \theta_n\tau_n\|\Delta_h\sigma_h^n\|^2\right) + \eta(1-\bar{\nu})\theta_n\tau_n\|\Delta_h\sigma_h^n\|^2\\
&+2C_3(1+\delta^*)(1+\bar{\nu})\tau_{n+1}\left(\|\sigma_h^{n+1}\|^2 + \|\sigma_h^n\|^2 + \|\sigma_h^{n-1}\|^2\right) + C\mathcal{R}^{n+1}.
\end{aligned} \tag{5.16}$$

This is exactly (5.1) if we make the identification $a_n = \|\sigma_h^n\|^2, b_n = (\delta^*+2)\|\sigma_h^n - \sigma_h^{n-1}\|^2, c_n = \|\Delta_h\sigma_h^n\|^2, C_4 = 2C_3(1+\Delta^*)(1+\bar{\nu})$.

In order to verify the remaining conditions of Lemma 5.1, we notice that

$$\|\sigma_h^{n+1}\|^2, (\delta^*+2)\|\sigma_h^{n+1}-\sigma_h^n\|^2, \|\Delta_h\sigma_h^{n+1}\|^2, \theta_{n+1}, \tau_{n+1}\mathcal{R}^{n+1} \ge 0.$$

In addition, by the time-step restriction (5.5), we have

$$\tau_{n+1} < \frac{1-\bar{\nu}}{4C_3(1+\delta^*)(1+\bar{\nu})(1+\gamma^*+(\gamma^*)^2)} = \frac{(1+2\gamma^*-(\gamma^*)^2)^2}{8C_3(1+2\gamma^*)(1+\gamma^*+(\gamma^*)^2)(1+\gamma^*)^2}.$$

For the initial step $\|\sigma_h^0\|^2 = 0$ and $\|\sigma_h^1 - \sigma_h^0\|^2 = \|\sigma_h^1\|^2$; then by Lemma 5.1 we have

$$\begin{aligned} &\|\sigma_h^{n+1}\|^2 + 2(\delta^*+2)\sum_{k=1}^{n}\|\sigma_h^{k+1}-\sigma_h^k\|^2 + 2\theta_{n+1}\tau_{n+1}\|\Delta_h\sigma_h^{n+1}\|^2 \\ &+ 2(1-\eta)\sum_{k=1}^{n-1}\theta_{k+1}\tau_{k+1}\|\Delta_h\sigma_h^{k+1}\|^2 \\ &\le \exp\left(\frac{4C_3(1+\delta^*)(1+\bar{\nu})(1+\gamma^*+(\gamma^*)^2)}{1-\bar{\nu}}\sum_{k=1}^{n}\tau_k\right)\mathcal{R}_n^{'}, \end{aligned} \tag{5.17}$$

where

$$\mathcal{R}_n^{'} = \frac{2+\bar{\nu}(2+\delta^*)}{1-\bar{\nu}}\|\sigma_h^1\|^2 + 2\left(\eta + \frac{2\bar{\nu}}{1-\bar{\nu}}\right)\theta_1\tau_1\|\Delta_h\sigma_h^1\|^2 + \frac{2C}{1-\bar{\nu}}\sum_{k=1}^{n}\mathcal{R}^{k+1}.$$

Here we use the fact that $\theta_1 = \frac{1}{2}\left(\varepsilon^2(1+\delta^*) + A\tau_1\right)\frac{\mu_1}{1-\lambda_1} < \varepsilon^2(1+\delta^*) + A\tau_1 < C\varepsilon^2$, so

$$\mathcal{R}_n^{'} \le C(\|\sigma_h^1\|^2 + \varepsilon^2\tau_1\|\Delta_h\sigma_h^1\|^2) + \frac{2C}{1-\bar{\nu}}\sum_{k=1}^{n}\mathcal{R}^{k+1} \le C\left(\mathcal{R}^1 + \sum_{k=1}^{n}\mathcal{R}^{k+1}\right) = C\mathcal{R}^*,$$

which is derived from the estimate of initial term (4.24). So we have

$$\|\sigma_h^{n+1}\|^2 \le C\mathcal{R}^*.$$

Combining the estimate for ρ^{n+1},

$$\|\rho^{n+1}\| \le Ch^{q+1}\|u^{n+1}\|_{H^{q+1}},$$

we finally obtain the optimal convergence analysis. Moreover, carefully checking the proof reveals that C in (5.6) depends on $T, \varepsilon, \gamma^*, \zeta$, and $E(u_h^0)$. ∎

Remark 5.1. We remark that the allowable value on *gamma** can be easily improved. Due to the continuity of the function $\ell(\zeta)$, the upper bound of γ^* can be close to

$$\ell(0) = \frac{2\sqrt{13}}{3}\cos\left(\frac{1}{3}\arccos\left(-\frac{8}{13\sqrt{13}}\right)\right) - \frac{2}{3} \approx 1.343$$

by choosing ζ small enough. For example, we may take $\gamma^* = 1.34 < \ell(0)$. There are other means to increase the allowable value of γ^*. In fact, we notice that the terms $\frac{7\varepsilon^2}{16}\left\|\Delta_h\sigma_h^{n+1}\right\|^2$ and $\frac{\varepsilon^2}{16\delta}\|\Delta_h\sigma_h^{n+1}\|^2$ in Lemma 4.4 come from the Cauchy–Schwarz inequality and Young's inequality. We can adjust the coefficients so that these terms become $s\frac{7\varepsilon^2}{16}\left\|\Delta_h\sigma_h^{n+1}\right\|^2$ and $s\frac{\varepsilon^2}{16\delta}\|\Delta_h\sigma_h^{n+1}\|^2$, where s is a constant small enough. In turn, the term $\left(\varepsilon^2(1+\delta) + A\tau_{n+1}\right)\mu_{n+1}\tau_{n+1}\|\Delta_h\sigma_h^{n+1}\|^2$ becomes $\left(\varepsilon^2(\chi+\delta) + A\tau_{n+1}\right)\mu_{n+1}\tau_{n+1}\|\Delta_h\sigma_h^{n+1}\|^2$ in (4.23), where χ is one constant smaller than 2 but close to 2. As a result, analogously to the derivation of (5.3), we may obtain a new equation $x^3 + 3x^2 - 5x - 3 = 0$. This new equation admits a root

$$\frac{4\sqrt{2}}{\sqrt{3}} \cos\left(\frac{1}{3} \arccos\left(-\frac{3\sqrt{3}}{8\sqrt{2}}\right)\right) - 1 \approx 1.53,$$

which could be a modified upper bound for γ^*.

6. Numerical results. In this section we report numerical results based on the fully discrete second order BDF scheme (2.6).

To check for accuracy, we consider a two-dimensional computational domain $\Omega = (0,1)^2$ with the following exact solution:

$$u_e(x, y, t) = \cos(\pi x) \cos(\pi y) \mathrm{e}^{-t}. \tag{6.1}$$

This implies that u_e satisfies the Cahn–Hilliard equation (1.2) with an artificial, time-dependent forcing term added on the right-hand side:

$$\partial_t u_e = \Delta(u_e^3 - u_e - \varepsilon^2 \Delta u_e) + g, \qquad (x, y, t) \in \Omega \times (0, T]. \tag{6.2}$$

The final time is set to be $T = 1$, and the physical parameter and the artificial constant are given by $\varepsilon^2 = 0.05$, $A = 1$. The nonlinear equations are solved by Newton's method. In the iteration process, the initial guess is chosen to be a second order extrapolation of the previous two steps, i.e., $u_h^{n+1,0} = (1 + \gamma_{n+1}) u_h^n - u_h^{n-1}$, which usually leads to one iteration stage fewer than the one with an initial guess as $u_h^{n+1,0} = u_h^n$. Therefore, this methodology reduces the computation cost. The stopping criterion for the nonlinear iteration is given by $\|u_h^{n+1,(m)} - u_h^{n+1,(m-1)}\| < h^3$. We compute numerical solutions with grid sizes $N_h = 16, 32, 64, 128, 256,\ 512$, with the L^2 errors reported at the final time $T = 1$.

6.1. Grid refinement strategy 1. For the initial time step size, we set $\tau_1 = h$. For the coarsest grid, we first generate a series of time nodes $\{t_n\}$ with uniform step sizes. Then we add a 10% perturbation onto $\{t_n\}$, obtaining new time-step series $\{\tau_n\}$. The grid refinement strategy is as follows: Denote by $\{t_n^{\text{coarse}}\}$ and $\{t_n^{\text{fine}}\}$ the time node series of the coarse grid and the fine grid, respectively. For each odd k, take $t_k^{\text{fine}} = \frac{1}{2} t_{(k+1)/2}^{\text{coarse}}$. For each even k, t_k^{fine} is set to be the average of t_{k+1}^{fine} and t_{k-1}^{fine}, with 10% perturbation. Such a random approach easily leads to large Γ_N. Figure 6.1 shows this refinement strategy.

Figure 6.2 shows the L^2 errors and the corresponding convergence orders between the numerical and exact solutions. A clear second order accuracy, for both the temporal and spatial approximations, is observed in the convergence test.

6.2. Grid refinement strategy 2. Define the time-step ratio $\gamma = 1.3$. The initial time-step is determined by $\tau_1 = \frac{3}{23(1.3^8 - 1)}$. For the coarsest grid, we divide the time step size series $\{\tau_n\}$ into two halves: $\tau_1, \tau_2, \ldots, t\tau_{N_T/2}$, and $\tau_{N_T/2+1}, \tau_{N_T/2+2}, \ldots, \tau_{N_T}$. In the first half, time step size τ_k is chosen to be γ times the previous time step size, i.e., $\tau_2 = \gamma\tau_1, \tau_3 = \gamma\tau_2, \ldots, \tau_{N_T/2} = \gamma\tau_{N_T/2-1}$. In the second half, τ_k is chosen to be $1/\gamma$ times the previous time step size, i.e., $\tau_{N_T/2+2} = \frac{1}{\gamma}\tau_{N_T/2+1}, \ldots, \tau_{N_T} = \frac{1}{\gamma}\tau_{N_T-1}$. Additionally, we set $\tau_{N_T/2+1} = \gamma\tau_{N_T/2}$. The grid refinement strategy is that we first divide by 2 the time step size series of the coarse grid and then put it in the first half of the time-step series of the fine grid. Finally, we duplicate the first half of

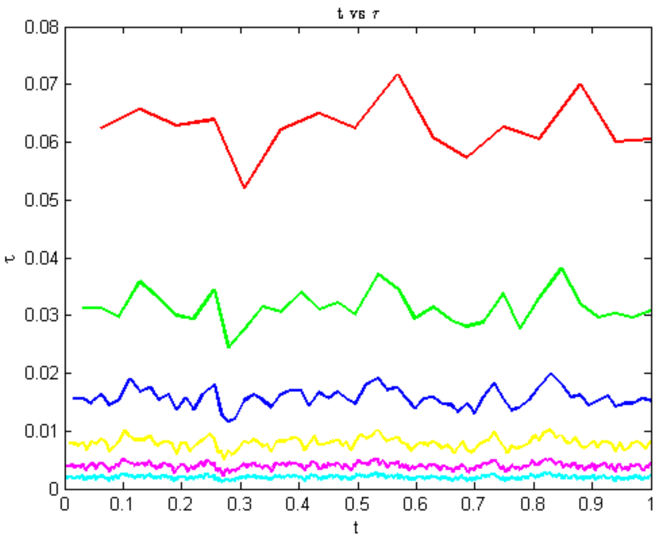

FIG. 6.1. *The curves from top to bottom represent the variable time-step with grid size* $N_h = 16$*,* $N_h = 32$*,* $N_h = 64$*,* $N_h = 128$*,* $N_h = 256$*, and* $N_h = 512$*.*

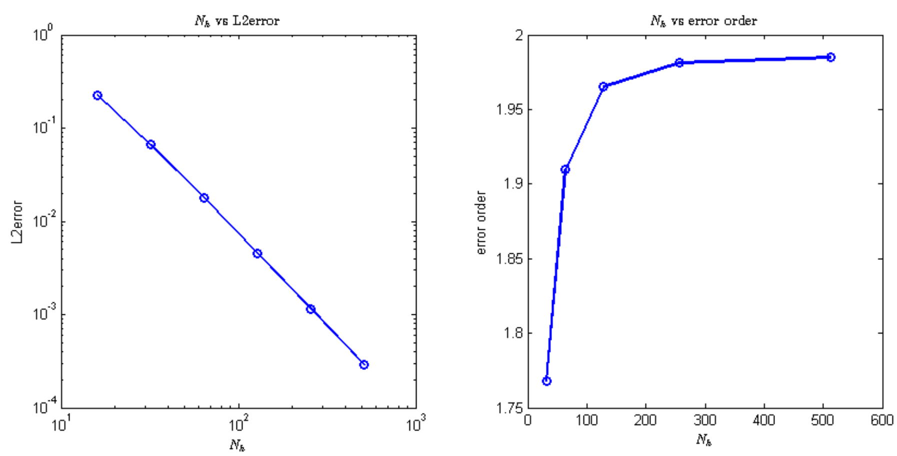

FIG. 6.2. L^2 *numerical errors at* $T = 1.0$ *and the corresponding convergence orders versus* N_h *(log-log plot) for the second order BDF scheme* (2.6)*. The surface diffusion parameter is taken to be* $\varepsilon^2 = 0.05$*.*

the time-step series of the fine grid to its second half in order to make the fine grid time-step series complete. Figure 6.3 shows this refinement strategy.

Figure 6.4 shows the L^2 errors and the corresponding convergence orders between the numerical and exact solutions. A clear second order accuracy, for both the temporal and spatial approximations, is observed in the convergence test.

In order to observe the dependence of the convergence rate on γ, we vary γ from

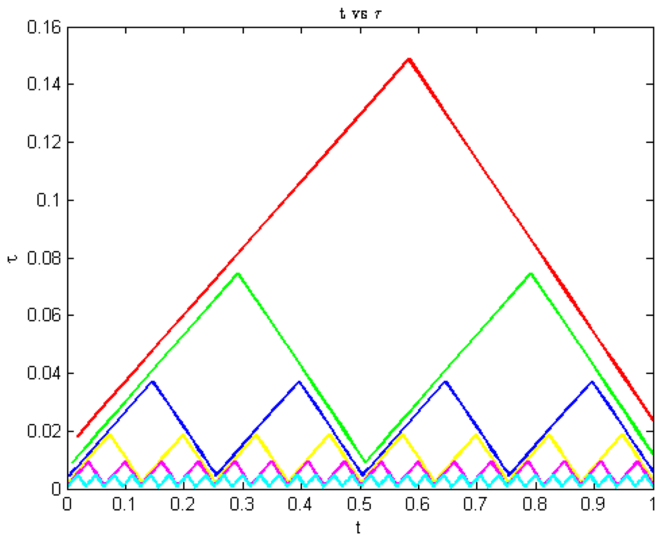

FIG. 6.3. *The lines from top to bottom represent the variable time-step with grid size* $N_h = 16$*,* $N_h = 32$*,* $N_h = 64$*,* $N_h = 128$*,* $N_h = 256$*, and* $N_h = 512$*.*

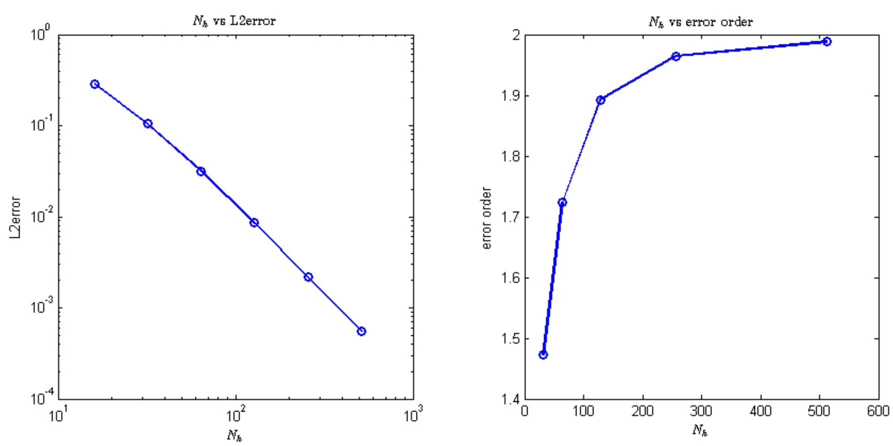

FIG. 6.4. L^2 *numerical errors at* $T = 1.0$ *plotted versus* N_h *(log-log plot) for the second order BDF scheme* (2.6)*. The surface diffusion parameter is taken to be* $\varepsilon^2 = 0.05$*.*

1.3 to 2.0 and introduce the following convergence orders:

$$order(i) = \frac{\log \frac{L2error(i)}{L2error(i+1)}}{\log \frac{N_h(i+1)}{N_h(i)}}, \quad 1 \le i \le 5.$$

Table 6.1 shows convergence orders under different choices of γ, with grid refinement strategy 2. It demonstrates the insensitive dependence on γ for the range considered.

6.3. Energy decay. Here we report numerical results on the decay of energy. Recall that when the interface width is much smaller than the domain size, the energy is expected to decay at the rate of $t^{-1/3}$ with a rigorous lower bound available in the

TABLE 6.1
Convergence order.

γ	$order(1)$	$order(2)$	$order(3)$	$order(4)$	$order(5)$
1.3	1.49848	1.72519	1.88947	1.9627	1.98763
1.4	1.41375	1.63429	1.8333	1.93577	1.97566
1.5	1.35521	1.55709	1.77916	1.90735	1.96236
1.6	1.3163	1.49276	1.72895	1.87884	1.94846
1.7	1.29022	1.43892	1.68309	1.851	1.93437
1.8	1.27158	1.39324	1.64145	1.82422	1.92037
1.9	1.25625	1.35388	1.60368	1.79871	1.90667
2.0	1.24077	1.31939	1.56936	1.77456	1.89336

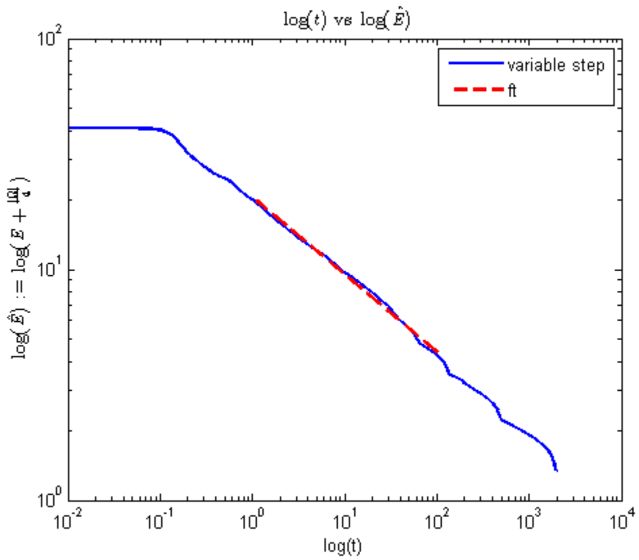

FIG. 6.5. *Log-log plot of the temporal evolution of the energy $\hat{E}$ for $\varepsilon^2 = 0.005$. The energy decreases like $t^{-\frac{1}{3}}$ until saturation. The blue line represents the energy plot obtained by the simulation, while the red line is obtained by least squares approximations to the energy data. The least squares fit is only taken for the linear part of the calculated data, only up to about time $t = 100$. The fitted line has the form at^b, with $a = 19.96$, $b = -0.3192$. (Color available online.)*

literature. We compare the numerical simulation result with the predicted energy decay rate, using the proposed second order BDF scheme (2.5) for the Cahn–Hilliard flow (1.2). The surface diffusion coefficient parameter is taken to be $\varepsilon^2 = 0.005$, and the computational domain is taken to be $\Omega = (0, 12.8)^2$, with a resolution of $N_h = 128$ for spatial discretization. As for the time grid, the strategy is to put a 10% perturbation to the previous step.

In order to make energy nonnegative all the time, we introduce the following modified energy by adding a constant to the original energy:

$$\hat{E}(u) = \int_\Omega \left(\frac{1}{4}u^4 - \frac{1}{2}u^2 + \frac{1}{4} + \frac{\varepsilon^2}{2}|\nabla u|^2\right) \mathrm{d}\mathbf{x} = E(u) + \frac{1}{4}|\Omega|. \tag{6.3}$$

Figure 6.5 presents the log-log plot for the energy versus time, with the given physical parameter $\varepsilon^2 = 0.005$. The detailed scaling "exponent" is obtained using least squares fits of the computed data up to time $t = 100$. A clear observation of the at^b scaling law can be made, with $a = 19.96$, $b = -0.3192$. Therefore, we have verified in our numerical simulation the energy dissipation law and the coarsening rate.

7. Concluding remarks. In this paper we have presented a second order variable time-step BDF scheme for the Cahn–Hilliard equation (1.2) in conjunction with a mixed finite element approximation in space. The scheme is uniquely solvable and unconditionally energy stable with mild assumptions on the time step size and the ratio of adjacent time-steps. Moreover, rigorous error estimates in the form of $\mathcal{O}(\tau^2 + h^2)$ in the $\ell^\infty(0, T; L^2)$ norm have been established without any undesirable exponential prefactor in Γ_n which is related to the number of transitions in the variable time-stepping. Such a rigorous result is new even in the linear case to the best of our knowledge. The proof relies on a novel generalized discrete Gronwall-type inequality that is able to deal with differences of nonnegative terms. In addition, the numerical experiment shows that the proposed second order BDF scheme is able to produce accurate long time numerical results with a reasonable computational cost. In particular, the energy dissipation rate given by the numerical simulation indicates an almost perfect match with the theoretical $t^{-1/3}$ prediction. Analysis of a truly adaptive strategy based on the variable stepping method as well as higher order methods is underway.

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