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A Second-Order Energy Stable BDF Numerical Scheme for the Viscous Cahn-Hilliard Equation with Logarithmic Flory-Huggins Potential

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Abstract. In this paper, a viscous Cahn-Hilliard equation with logarithmic Flory-Huggins energy potential is solved numerically by using a convex splitting scheme. This numerical scheme is based on the Backward Differentiation Formula (BDF) method in time and mixed finite element method in space. A regularization procedure is applied to logarithmic potential, which makes the domain of the regularized function $F(u)$ to be extended from $(-1,1)$ to $(-\infty,\infty)$. The unconditional energy stability is obtained in the sense that a modified energy is non-increasing. By a carefully theoretical analysis and numerical calculations, we derive discrete error estimates. Subsequently, some numerical examples are carried out to demonstrate the validity of the proposed method.

AMS subject classifications: 65N30

Key words: Viscous Cahn-Hilliard, logarithmic potential, BDF scheme, error estimates.

1 Introduction

The Cahn-Hilliard (CH) equation which was first introduced by Cahn-Hilliard [1–3] describes the phase separation and coarsening phenomena in non-uniform systems such as alloys, glasses and polymer mixtures. The Cahn-Hilliard equation has been used as a model for various problems, whose applications are very extensive. We review some physical and industrial applications of Cahn-Hilliard model: microphase separation of diblock copolymers [4]; spinodal decomposition [5]; image inpainting [6]; phase-field modeling of tumor growth [7]; volume reconstruction [8]; topology optimization [9]; co-continuous binary polymer microstructures [10]; microstructures with elastic inhomogeneity [11], and multiphase fluid flows [12–14].

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Numerical methods for solving the Cahn-Hilliard equation provide an important tool for studying the dynamics described by the Cahn-Hilliard system, which have been extensively investigated. For the spatial discretization, a series of methods have been developed and applied. Finite difference methods and spectral methods [15–17] were proposed for rectangular regions. The finite element method can be used for the general domain of complex geometries [18–20]. Non-conforming elements or discontinuous Galerkin methods were proposed in [21–24]. For time discretization, energy stable methods have attracted more and more attention in the study of Cahn-Hilliard equations. Convex splitting method [25–27] is a very effective energy stable method, which is usually nonlinear. Stabilized semi-implicit methods [28–30] are linear schemes, which are also energy stable. A technique called Invariant Energy Quadratization (IEQ) which was successfully applied to different phase-field models by authors [31], was extended to handle the Cahn-Hilliard equation in [32, 33]. By introducing a scalar auxiliary variable (SAV), Shenjie [34] proposed a numerical technique to deal with nonlinear terms in gradient flows, which construct efficient and robust energy stable schemes for a large class of gradient flows [35, 36]. Exponential time differencing (ETD) method whose approximation is stabilized semi-implicit methods has been used in solving phase field equations [37, 38]. It is notice that the convex splitting method with nonlinear scheme is more accurate in comparison to above mentioned linear schemes.

The most of developed numerical algorithms mainly focused on the discretization of the polynomial potential for the Cahn-Hilliard equation. However, the free energy with the logarithmic potential is often considered to be more physically realistic than that with a polynomial free energy, because the former is derived from regular or ideal solution theories [39]. Dong and Wang et al. [40, 41] presented finite difference numerical scheme for the Cahn-Hilliard equation with a logarithmic Flory Huggins energy potential, which is unconditionally stabile and gave error estimates. Thomas P. Witelski [42] focused on the discussion of important qualitative features of the solutions of the nonlinear singular Cahn-Hilliard equation with degenerate mobility for the Flory-Huggins-deGennes free energy model. John and James [43] presented finite element method of the Cahn-Hilliard equation with a logarithmic free energy and non-degenerate concentration dependent mobility. Recently. Du et al. [44] discussed Allen-Cahn equation with logarithmic Flory-Huggins Potential based on ETD scheme, which could preserve maximum bound principle of Allen-Cahn type phase field equations and has applied to the Cahn-Hilliard [45] equation and epitaxial thin film equations [37]. More numerical methods for phase-field equations with logarithmic Flory-Huggins Potential can be also found in [46, 47].

Recently, researchers have devoted tremendous efforts to the relaxed Cahn-Hilliard equation, i.e., the viscous Cahn-Hilliard equation. Formally, the governing equation of the viscous Cahn-Hilliard equation is slightly different from the Cahn-Hilliard equation by incorporating one extra terms i.e., a strong damping (or viscosity) term. The viscous term was first proposed by Novick-Cohen [48] in order to introduce an additional regularity and some parabolic smoothing. It can be viewed as a singular limit of the phase field equations for phase transitions [49]. Significantly despite a great deal of work was done for the numerical solution of the classical Cahn-Hilliard equation, almost all researches related to the viscous Cahn-Hilliard equation were focused on the theoretical PDE analysis with very few algorithm design or numerical analysis. This is due to the numerical difficulties of proper discretization for the viscous effect. Choi and Kim [50] presented an unconditionally stable finite difference method for solving the viscous Cahn-Hilliard equation. The numerical approximations of the viscous Cahn-Hilliard equation with the hyperbolic relaxation is considered by Yang and Zhao in [51]. Colli and Farshbaf-Shaker et al. [52] investigated optimal boundary control problems for the viscous Cahn-Hilliard variational inequalities with a dynamic boundary condition involving double obstacle potentials and the Laplace-Beltrami operator. Therefore, a more efficient and accurate time marching scheme is required.

Our work is to solve the viscous Cahn-Hilliard equation

$$u_t=\Delta w \qquad \text{in } \Omega\times(0,T], \tag{1.1a}$$

$$w=f(u)-\varepsilon^2\Delta u+\beta u_t \qquad \text{in } \Omega\times(0,T], \tag{1.1b}$$

$$\partial_n u=\partial_n w=0 \qquad \text{on } \partial\Omega\times(0,T], \tag{1.1c}$$

$$u(\cdot,0)=u_0 \qquad \text{in } \Omega. \tag{1.1d}$$

Here $\Omega\subset R^d$, $d=2,3$ be an open polygonal or polyhedral domain with a Lipschitz continuous boundary $\partial\Omega$, n is the unite outward normal of the boundary, ε is a constant measuring the thickness of the transition layer, $\beta>0$ is the viscosity parameter (it becomes the classical Cahn-Hilliard system when $\beta=0$), f is the derivative of a logarithmic Flory-Huggins energy potential F, which is defined as

$$F(u)=\frac{\theta}{2}((1+u)\ln(1+u)+(1-u)\ln(1-u))+\frac{1}{2}(1-u^2), \quad u\in(-1,1), \tag{1.2}$$

where satisfied $\theta<1$.

The energy of the viscous Cahn-Hilliard equation is given by

$$E=\int_\Omega\Big(\frac{\varepsilon^2}{2}|\nabla u|^2+F(u)\Big)dx. \tag{1.3}$$

The viscous Cahn-Hilliard equation is mass conservative, i.e., $(u(\cdot,t),1)=(u_0,1)$ and energy dissipative

$$\frac{dE}{dt}=-\int_\Omega|\nabla\mu|^2dx\leq 0, \tag{1.4}$$

where $(\cdot,\cdot)$ is the standard L^2 inner product over Ω.

As we all know, temporal second-order numerical method is much more accurate efficient than the first-order counterparts. It is more challenging than the first-order ones. Devoting to second order temporal accuracy, we use the implicit backward differentiation formula (BDF) method and present a second-order finite scheme for the viscous

Cahn-Hilliard equation with logarithmic Flory-Huggins energy potential. In fact, BDF scheme has attracted a great deal of attention in recent year. Yan et al. [53] presented a second order accurate energy stable numerical scheme for the Cahn-Hilliard equation, with a mixed finite element approximation in space. Chen et al. [54]analyzed finite difference numerical schemes for the Cahn-Hilliard equation. Zhang et al. [55] compared the modified-energy stable SAV-Type schemes and classical BDF methods on Benchmark problems for the Functionalized Cahn-Hilliard Equation. Chen et al. [56]proposed a second order in time variable step BDF2 numerical scheme for the Cahn-Hilliard equation.

The rest of the article is organized as follows. The theoretical preparation and discrete finite element scheme are reviewed in Section 2. The unique solvability is proven in Section 3. In Section 4 we show the fully discrete scheme is energy stable. The detailed error estimate is given in Section 5. Numerical evidences showing the convergence and efficiency of the scheme are provided in Section 6. Conclusions are drawn in Section 7.

2 Theoretical preparation and the discrete scheme

2.1 Theoretical preparation

In this subsection, some notations and lemmas are given for subsequent proofs. We denote

$$(u,v)=\int_\Omega u(x)v(x)dx,\quad \|u\|=\|u\|_{L^2(\Omega)},\quad \|u\|_{H^1}=\Big(\int_\Omega |u|^2dx+\int_\Omega |Du|^2dx\Big)^{\frac{1}{2}}.$$

Let N be a positive integer and $0=t_0<t_1<\cdots<t_N=T$ be a uniform partition of $[0,T]$. $\tau=:t_{n+1}-t_n$, $n=0,1,\cdots,N$ is the time step size. Let $u^n=u(\cdot,t_n)$, then the second-order in time BDF method [57] for $n\geq 1$ reads

$$D_\tau u^{n+1}=\frac{3u^{n+1}-4u^n+u^{n-1}}{2\tau}, \tag{2.1}$$

and for the first time level we use the backward Euler approximation

$$\delta_\tau u^1=\frac{u^1-u^0}{\tau}. \tag{2.2}$$

Lemma 2.1 ([58]). *For sufficiently smooth function $u(t)=u(\cdot,t)\in C^3[0,T]$, the above approximation of first-order derivative at time t_{n+1} is of second-order convergence, i.e.,*

$$u_t^{n+1}=D_\tau u^{n+1}+R_t^{n+1},\quad n\geq 1, \tag{2.3a}$$

$$u_t^1=\delta_\tau u^1+E_1,\qquad n=0, \tag{2.3b}$$

$$\|R_t^{n+1}\|\leq C\tau^2\max_{t\in[0,T]}\|u_{ttt}\|,\quad \|E_1\|\leq C\tau^2\max_{t\in[0,T]}\|u_{ttt}\|, \tag{2.3c}$$

with the constant C independent of τ.

We use the Elliott and Luckhaus regularization for our problem, with the logarithmic free energy $F(u)$ replaced by the twice continuously differentiable function $\check{F}(u)$

$$\check{F}=:\begin{cases}\frac{\theta}{2}(1+u)\ln(1+u)+\frac{\theta}{4k}(1-u)^2+\frac{\theta}{2}(1-u)\ln k-\frac{\theta k}{4}+\frac{1}{2}(1-u^2), & u\geq 1-k,\\ F(u), & |u|<1-k,\\ \frac{\theta}{2}(1-u)\ln(1-u)+\frac{\theta}{4k}(1+u)^2+\frac{\theta}{2}(1+u)\ln k-\frac{\theta k}{4}+\frac{1}{2}(1-u^2), & u\leq -1+k,\end{cases}$$

where $k\in(0,1)$. The monotone function

$$\check{f}(u)=:\check{F}'(u)=\begin{cases}\frac{\theta}{2}\ln(1+u)+\frac{\theta}{2}-\frac{\theta}{2k}(1-u)-\frac{\theta}{2}\ln k-u, & u\geq 1-k,\\ \frac{\theta}{2}(\ln(1+u)-\ln(1-u))-u, & |u|<1-k,\\ -\frac{\theta}{2}\ln(1-u)-\frac{\theta}{2}+\frac{\theta}{2k}(1+u)+\frac{\theta}{2}\ln k-u, & u\geq -1+k.\end{cases}$$

Hereinafter, f and F will be substituted by $\check{F}$ and $\check{f}$ in our analysis. However, for convenience, the ˇ will be omitted.

2.2 A semi-discrete numerical scheme

The weak formulation of the viscous Cahn-Hilliard equation can be written as

$$(u_t,v)+(\nabla w,\nabla v)=0, \qquad \forall v\in H^1(\Omega), \tag{2.4a}$$
$$(w,\psi)-(f(u),\psi)-\varepsilon^2(\nabla u,\nabla\psi)-\beta(u_t,\psi)=0, \qquad \forall\psi\in H^1(\Omega), \tag{2.4b}$$

with initial condition $u(t=0)=u_0$ and $f(u)=f_1(u)-f_2(u)$, where

$$f_1(u)=:\begin{cases}\frac{\theta}{2}\ln(1+u)+\frac{\theta}{2}-\frac{\theta}{2k}(1-u)-\frac{\theta}{2}\ln k, & u\geq 1-k,\\ \frac{\theta}{2}(\ln(1+u)-\ln(1-u)), & |u|<1-k,\\ -\frac{\theta}{2}\ln(1-u)-\frac{\theta}{2}+\frac{\theta}{2k}(1+u)+\frac{\theta}{2}\ln k, & u\leq -1+k,\end{cases}$$
$$f_2(u)=:u.$$

From the definition of f_1 and f_2, we can easily prove that

$$0<f_1'(u)\leq L=:\frac{\theta}{(2-k)k}, \quad \forall u\in(-\infty,\infty) \quad \text{and} \quad f_2'(u)=1>0.$$

The semi-discrete second-order splitting scheme for the viscous Cahn-Hilliard equation can be written as follows. For $n\geq 1$, given u^n, u^{n-1}, seek (u^{n+1},w^{n+1}) such that

$$(D_\tau u^{n+1}),v)+(\nabla w^{n+1},\nabla v)=0, \tag{2.5a}$$
$$(w^{n+1},\psi)-(f_1(u^{n+1})-f_2(u^n,u^{n-1}),\psi)-\varepsilon^2(\nabla u^{n+1},\nabla\psi)-\beta(D_\tau u^{n+1},\psi)=0, \tag{2.5b}$$

where $f_2(u^n,u^{n-1})=2u^n-u^{n-1}$.

We use a standard first-order energy stable method to obtain u^1, w^1 as follows for the initialization: given u^0, find u^1, w^1, such that

$$\Big(\frac{u^1-u^0}{\tau},v\Big)+(\nabla w^1,\nabla v)=0, \tag{2.6a}$$

$$(w^1,\psi)-(f_1(u^1)-f_2(u^0),\psi)-\varepsilon^2(\nabla u^1,\nabla\psi)-\beta\Big(\frac{u^1-u^0}{\tau},\psi\Big)=0. \tag{2.6b}$$

Let $F_1(u)$ and $F_2(u)$ denote the corresponding parts of f_1 and f_2 in the definition of $F(u)$. Then by the Taylor expansion and the facts that $F_1'(u)=f_1(u)$ and $F_1''(u)=f_1'(u)>0$, we have: for some $\rho\in[u^n,u^{n+1}]$

$$\begin{aligned}F_1(u^n)-F_1(u^{n+1})=&F_1'(u^{n+1})(u^n-u^{n+1})+\frac{1}{2}F_1''(\rho)(u^n-u^{n+1})^2\\ \geq& f_1(u^{n+1})(u^n-u^{n+1}).\end{aligned} \tag{2.7}$$

For f_2,

$$\begin{aligned}&-f_2(u^n,u^{n-1})(u^{n+1}-u^n)\\ =&-(2u^n-u^{n-1},u^{n+1}-u^n)\\ =&-(u^n,u^{n+1}-u^n)-(u^n-u^{n-1},u^{n+1}-u^n)\\ =&-\frac{1}{2}(\|u^{n+1}\|^2-\|u^n\|^2)+\frac{1}{2}\|u^{n+1}-u^n\|^2\\ &+(u^{n+1}-2u^n+u^{n-1},u^{n+1}-u^n)-\|u^{n+1}-u^n\|^2\\ =&-\frac{1}{2}\|u^{n+1}\|^2+\frac{1}{2}\|u^{n+1}-u^n\|^2-\Big(-\frac{1}{2}\|u^n\|^2+\frac{1}{2}\|u^n-u^{n-1}\|^2\Big)\\ &+\frac{1}{2}\|u^{n+1}-2u^n+u^{n-1}\|^2-\frac{1}{2}\|u^{n+1}-u^n\|^2.\end{aligned} \tag{2.8}$$

A combination (2.7) and (2.8), we obtain

$$\begin{aligned}&F(u^{n+1})-F(u^n)+\frac{1}{2}\|u^{n+1}-u^n\|^2-\frac{1}{2}\|u^n-u^{n-1}\|^2-\frac{1}{2}\|u^{n+1}-u^n\|^2\\ \leq&(f_1(u^{n+1})-f_2(u^n,u^{n-1}))(u^{n+1}-u^n).\end{aligned} \tag{2.9}$$

2.3 Fully discrete numerical scheme

Let $T_h=\{K\}$ be a conforming, shape-regular, globally quasi-uniform family of triangulation of Ω. For a nonnegative integer q', define the piecewise polynomial space $S_h=\{v_h\in C(\Omega)|v_h|_K\in P_{q'}(x,y),\ \forall K\in T_h\}\subset H^1(\Omega)$, where $P_{q'}(x,y)$ is the set of polynomials of x, y with the degree no greater than q'. In addition, we define

$$L_0^2=:\{u\in L^2(\Omega)|(u,1)=0\}\quad\text{and}\quad \hat{S}_h=:S_h\cap L_0^2(\Omega).$$

The fully discrete finite element formulation for the viscous Cahn-Hilliard equation can be written as follows. For $n\geq 1$, $\forall(v_h,\psi_h)\in S_h\times S_h$, given $u_h^n,u_h^{n-1}\in S_h$, seek $(u_h^{n+1},w_h^{n+1})\in S_h\times S_h$ such that

$$\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},v_h\Big)+(\nabla w_h^{n+1},\nabla v_h)=0, \tag{2.10a}$$

$$(w_h^{n+1},\psi_h)-(f_1(u_h^{n+1})-f_2(u_h^n,u_h^{n-1}),\psi_h)-\varepsilon^2(\nabla u_h^{n+1},\nabla\psi_h)$$
$$-\beta\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},\psi_h\Big)=0. \tag{2.10b}$$

In order to ensure the unique solvability of the scheme, an additional term $A\tau\Delta(u^{n+1}-u^n)$, $(A\geq\frac{1}{16})$ is added, then we have

$$\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},v_h\Big)+(\nabla w_h^{n+1},\nabla v_h)=0, \tag{2.11a}$$

$$(w_h^{n+1},\psi_h)-(f_1(u_h^{n+1})-f_2(u_h^n,u_h^{n-1}),\psi_h)-\varepsilon^2(\nabla u_h^{n+1},\nabla\psi_h)$$
$$-A\tau(\nabla(u_h^{n+1}-u_h^n),\nabla\psi_h)-\beta\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},\psi_h\Big)=0. \tag{2.11b}$$

The scheme requires an initialization step. To this end, we introduce the Ritz Projection operator $R_h:H^1(\Omega)\to S_h$, satisfying

$$(\nabla(R_hu-u),\nabla\chi)=0,\quad \forall\chi\in S_h,\quad (R_hu-u,1)=0. \tag{2.12}$$

A standard first-order energy stable method is used to obtain $u_h^1,w_h^1\in S_h$ for the initialization as follows: given $u_h^0\in S_h$, find $u_h^1,w_h^1\in S_h$, such that

$$\Big(\frac{u_h^1-u_h^0}{\tau},v_h\Big)+(\nabla w_h^1,\nabla v_h)=0, \tag{2.13a}$$

$$(w_h^1,\psi_h)-(f_1(u_h^1)-f_2(u_h^0),\psi_h)-\varepsilon^2(\nabla u_h^1,\nabla\psi_h)-\beta\Big(\frac{u_h^1-u_h^0}{\tau},\psi_h\Big)=0, \tag{2.13b}$$

where $u_h^0=R_hu_0$.

3 Unique solvability

In this subsection, some definitions and lemma are given to prove that our scheme is unique solvability.

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

$$(\Delta_hv_h,\chi)=-(\nabla v_h,\nabla\chi),\quad \forall\chi\in S_h.$$

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

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

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

$$\|v_h\|_{-1,h}=:\sqrt{(v_h,(-\Delta_h)^{-1}v_h)}=\sup_{0\neq\chi\in\hat{S}_h}\frac{(v,\chi)}{\|\nabla\chi\|},\quad \forall v_h\in\hat{S}_h.$$

Lemma 3.1 ([59])**.** *Suppose $\chi,\psi\in\hat{S}_h(\Omega)$ and set*

$$(\chi,\psi)_{-1,h}=:(\nabla T_h(\chi),\nabla T_h(\psi))=(\chi,T_h(\psi))=(T_h(\chi),\psi). \tag{3.1}$$

Where $T_h:\hat{S}_h(\Omega)\to\hat{S}_h(\Omega)$ is the invertible linear operator, which is defined via the following variational problem: given $\chi\in\hat{S}_h(\Omega)$, find $T_h(\chi)\in\hat{S}_h(\Omega)$ such that

$$(\nabla T_h(\chi),\nabla\nu)=(\chi,\nu),$$

$(\cdot,\cdot)_{-1,h}$ defines an inner product on $\hat{S}_h(\Omega)$. Consequently, for all $\chi\in\hat{S}_h(\Omega)$ and $g\in S_h(\Omega)$,

$$|(\chi,g)|\leq\|\chi\|_{-1,h}\|\nabla g\|. \tag{3.2}$$

The following the Poincaré-type estimate holds

$$\|\chi\|_{-1,h}\leq C\|\chi\| \tag{3.3}$$

for some constant $C>0$.

Assuming that $\psi_h\in\hat{S}_h$, we take the test function as $v_h=(-\Delta_h)^{-1}\psi_h$ in our mixed scheme (2.11a)-(2.11b), then we obtain

$$\begin{aligned}&\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},(-\Delta_h)^{-1}\psi_h\Big)+\varepsilon^2(\nabla u_h^{n+1},\nabla\psi_h)\\&\quad+(f_1(u_h^{n+1})-f_2(u_h^n,u_h^{n-1})),\psi_h)+A\tau(\nabla(u_h^{n+1}-u_h^n),\nabla\psi_h)\\&\quad+\beta\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},\psi_h\Big)=0.\end{aligned} \tag{3.4}$$

By rearranging the above equation, for every $\psi_h\in\hat{S}_h$, we get

$$\begin{aligned}&\Big(f_1(u_h^{n+1})-(A\tau+\varepsilon^2)\Delta_h u_h^{n+1}+\frac{3}{2\tau}(-\Delta_h)^{-1}(u_h^{n+1}-\bar{u})+\frac{3\beta}{2\tau}(u_h^{n+1}-\bar{u}),\psi_h\Big)\\&=f[u_h^n,u_h^{n-1}](\psi_h),\end{aligned} \tag{3.5}$$

where $f[u_h^n,u_h^{n-1}]$ is a bounded linear functional involving the previous time iterates and $\bar{u}$ is the time-invariant mass average of u_h^k. We make the transformation $q_h=u_h^{k+1}-\bar{u}\in\hat{S}_h$. Then $q_h\in\hat{S}_h$ satisfies

$$\begin{aligned}&\Big(f_1(q_h+\bar{u})-(A\tau+\varepsilon^2)\Delta_h q_h+\frac{3}{2\tau}(-\Delta_h)^{-1}q_h+\frac{3\beta}{2\tau}q_h,\psi_h\Big)\\ =&f[u_h^n,u_h^{n-1}](\psi_h),\end{aligned} \tag{3.6}$$

iff $u_h^{k+1}\in\hat{S}_h$ satisfies (3.5). Define

$$\begin{aligned}G(q_h)=:&\frac{1}{2}\|F_1(q_h+\bar{u})\|^2+\frac{1}{2}(A\tau+\varepsilon^2)\|\nabla q_h\|^2\\ &+\frac{3}{4\tau}\|q_h\|_{-1,h}^2+\frac{3\beta}{4\tau}\|q_h\|^2-f[u_h^n,u_h^{n-1}](q_h).\end{aligned} \tag{3.7}$$

Since $G(q_h)$ is a strictly convex functional over the admissible set $\hat{S}_h$, it has a unique minimizer. The unique minimizer, $q_h\in\hat{S}_h$, satisfies the Euler-Lagrange equation, which coincides with the variational problem (3.6). By equivalence, the solution of (3.4) exists and is unique. The unique solvability of the initialisation scheme (2.13a)-(2.13b) can be established analogously.

4 The analysis of stability

4.1 Stability of the fully discrete scheme

The following energy stability estimates is available.

Theorem 4.1. *Let* (u_h^{n+1},w_h^{n+1}) *be the unique solution of the scheme* (2.11a)-(2.11b). *For any* $\tau,h,\varepsilon>0$, $n\geq 1$, *define*

$$\Xi(u_h^{n+1},u_h^n)=:E(u_h^{n+1})+\frac{1}{4\tau}\|u_h^{n+1}-u_h^n\|_{-1,h}^2+\frac{1}{2}\|u_h^{n+1}-u_h^n\|^2+\frac{\beta}{4\tau}\|u_h^{n+1}-u_h^n\|^2, \tag{4.1}$$

then the numerical scheme (2.11a)-(2.11b) *satisfies a energy law*

$$\Xi(u_h^{n+1},u_h^n)+\tau\Big(A-\frac{1}{16}\Big)\|\nabla u_h^{n+1}-\nabla u_h^n\|^2\leq\Xi(u_h^n,u_h^{n-1}), \tag{4.2}$$

where $A\geq\frac{1}{16}$.

Proof. Replacing v_h by $(-\Delta_h^{-1})(u_h^{n+1}-u_h^n)$ in (2.11a), which can be rewritten as

$$\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},-\Delta_h^{-1}(u_h^{n+1}-u_h^n)\Big)+(\nabla w_h^{n+1},\nabla(-\Delta_h^{-1})(u_h^{n+1}-u_h^n))=0, \tag{4.3}$$

with the deformation of first term on the left-hand side in (4.3)

$$\begin{aligned}&\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},(-\Delta_h^{-1})(u_h^{n+1}-u_h^n)\Big)\\ =&\tau\Big(\frac{5}{4}\Big\|\frac{u_h^{n+1}-u_h^n}{\tau}\Big\|_{-1,h}^2-\frac{1}{4}\Big\|\frac{u_h^n-u_h^{n-1}}{\tau}\Big\|_{-1,h}^2\Big)+\frac{\tau^3}{4}\Big\|\frac{u_h^{n+1}-2u_h^n+u_h^{n-1}}{\tau^2}\Big\|_{-1,h}^2. \end{aligned} \tag{4.4}$$

Taking $\psi_h=-(u_h^{n+1}-u_h^n)$ in (2.11b), we arrive at

$$\begin{aligned}&-(w_h^{n+1},u_h^{n+1}-u_h^n)+(f_1(u_h^{n+1})-f_2(u_h^n,u_h^{n-1}),u_h^{n+1}-u_h^n)\\ &\quad+\varepsilon^2(\nabla u_h^{n+1},\nabla(u_h^{n+1}-u_h^n))+A\tau\|\nabla u_h^{n+1}-\nabla u_h^n\|^2\\ &\quad+\beta\tau\Big(\frac{5}{4}\Big\|\frac{u_h^{n+1}-u_h^n}{\tau}\Big\|^2-\frac{1}{4}\Big\|\frac{u_h^n-u_h^{n-1}}{\tau}\Big\|^2\Big)+\frac{\beta\tau^3}{4}\Big\|\frac{u_h^{n+1}-2u_h^n+u_h^{n-1}}{\tau^2}\Big\|^2=0. \end{aligned} \tag{4.5}$$

Considering that (2.9), we yields

$$\begin{aligned}&-(w_h^{n+1},u_h^{n+1}-u_h^n)+(F(u_h^{n+1})-F(u_h^n),1)\\ &\quad+\frac{1}{2}\|u_h^{n+1}-u_h^n\|^2-\frac{1}{2}\|u_h^n-u_h^{n-1}\|^2-\frac{1}{2}\|u_h^{n+1}-u_h^n\|^2+\frac{\varepsilon^2}{2}(\|\nabla u_h^{n+1}\|^2-\|\nabla u_h^n\|^2)\\ &\quad+A\tau\|\nabla u_h^{n+1}-\nabla u_h^n\|^2+\beta\tau\Big(\frac{1}{4}\Big\|\frac{u_h^{n+1}-u_h^n}{\tau}\|^2-\frac{1}{4}\Big\|\frac{u_h^n-u_h^{n-1}}{\tau}\|^2\Big)\le 0. \end{aligned} \tag{4.6}$$

Summing (4.3) and (4.6) implies that

$$\begin{aligned}&\frac{1}{\tau}\|u_h^{n+1}-u_h^n\|_{-1,h}^2+\Xi(u_h^{n+1},u_h^n)-\Xi(u_h^n,u_h^{n-1})\\ &\quad-\frac{1}{2}\|u_h^{n+1}-u_h^n\|^2+A\tau\|\nabla u_h^{n+1}-\nabla u_h^n\|^2\le 0, \end{aligned} \tag{4.7}$$

with

$$\begin{aligned}\frac{1}{2}\|u_h^{n+1}-u_h^n\|^2&\le\frac{1}{2}\|\nabla u_h^{n+1}-\nabla u_h^n\|\cdot\|u_h^{n+1}-u_h^n\|_{-1,h}\\ &\le\frac{\tau}{16}\|\nabla u_h^{n+1}-\nabla u_h^n\|^2+\frac{1}{\tau}\|u_h^{n+1}-u_h^n\|_{-1,h}^2. \end{aligned} \tag{4.8}$$

The following result can be obtained

$$\Xi(u_h^{n+1},u_h^n)+\tau\Big(A-\frac{1}{16}\Big)\|\nabla u_h^{n+1}-\nabla u_h^n\|^2\le\Xi(u_h^n,u_h^{n-1}). \tag{4.9}$$

Thus, we completed the proof. □

Theorem 4.2. *The initialization scheme* (2.13a)-(2.13b) *enjoys the energy-decay property*

$$E(u_h^1)+\frac{1}{\tau}\|u_h^1-u_h^0\|_{-1,h}^2+\frac{\beta}{\tau}\|u_h^1-u_h^0\|^2\le E(u_h^0). \tag{4.10}$$

Proof. Replaced v_h by $(-\Delta_h^{-1})(u_h^1-u_h^0)$ in (2.13a), it can be rewritten as

$$\frac{1}{\tau}\|u_h^1-u_h^0\|_{-1,h}^2+(w_h^1,u_h^1-u_h^0)=0. \tag{4.11}$$

Taking $\psi_h=-(u_h^1-u_h^0)$ in (2.13b), we arrive at

$$\begin{aligned}&-(w_h^1,u_h^1-u_h^0)+(f_1(u_h^1)-f_2(u_h^0),u_h^1-u_h^0)\\&\quad+\varepsilon^2(\nabla u_h^1,\nabla(u_h^1-u_h^0))+\frac{\beta}{\tau}\|u_h^1-u_h^0\|^2=0.\end{aligned} \tag{4.12}$$

Using Taylor expansion, we have

$$(F(u^1)-F(u^0),1)\leq(f_1(u^1)-f_2(u^0),u^1-u^0). \tag{4.13}$$

Furthermore

$$\begin{aligned}&-(w_h^1,u_h^1-u_h^0)+(F(u_h^1)-F(u_h^0),1)\\&\quad+\frac{\varepsilon^2}{2}(\|\nabla u_h^1\|^2-\|\nabla u_h^0\|^2)+\frac{\beta}{\tau}\|u_h^1-u_h^0\|^2\leq 0.\end{aligned} \tag{4.14}$$

Adding (4.11) and (4.14), we deduce that

$$\frac{1}{\tau}\|u_h^1-u_h^0\|_{-1,h}^2+(F(u_h^1)-F(u_h^0),1)+\frac{\varepsilon^2}{2}(\|\nabla u_h^1\|^2-\|\nabla u_h^0\|^2)+\frac{\beta}{\tau}\|u_h^1-u_h^0\|^2\leq 0. \tag{4.15}$$

The proof is completed. □

Theorem 4.3. *Assume that $E(u_h^0)<C_0$, independent of h, τ, and there is a constant $C>0$ independent of h, τ such that the following estimates hold for any $h,\tau>0$,*

$$\|\nabla u_h^{n+1}\|^2\leq C, \tag{4.16a}$$

$$\frac{1}{\tau}\|u_h^{n+1}-u_h^n\|_{-1,h}^2\leq C, \tag{4.16b}$$

$$\tau\|\nabla w_h^{n+1}\|^2\leq C. \tag{4.16c}$$

Proof. According to Theorems 4.1 and 4.2, we can get the results of (4.16a) and (4.16b), directly. Taking $v_h=\tau w_h^{n+1}$ in (2.11a) and using Lemma 3.1 yield that

$$\begin{aligned}\tau\|\nabla w_h^{n+1}\|^2&=-\tau\Big(\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau},w_h^{n+1}\Big)\\&\leq\tau\Big\|\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau}\Big\|_{-1,h}\|\nabla w_h^{n+1}\|\\&\leq\frac{\tau}{2}\Big\|\frac{3u_h^{n+1}-4u_h^n+u_h^{n-1}}{2\tau}\Big\|_{-1,h}^2+\frac{\tau}{2}\|\nabla w_h^{n+1}\|^2\\&\leq\tau\Big\|\frac{3(u_h^{n+1}-u_h^n)}{2\tau}\Big\|_{-1,h}^2+\tau\Big\|\frac{(u_h^n-u_h^{n-1})}{2\tau}\Big\|_{-1,h}^2+\frac{\tau}{2}\|\nabla w_h^{n+1}\|.\end{aligned} \tag{4.17}$$

With (4.16b), we have

$$\frac{\tau}{2}\|\nabla w_h^{n+1}\| \leq C.$$

Thus, we complete the proof. □

5 Error analysis

5.1 Preliminary estimates

In this subsection, for the error estimates, we have the following regularity assumptions on the weak solutions

$$u \in H^1(0,T;H^{q+1}(\Omega)) \cap W^{1,\infty}(0,T,H^{q+1}), \tag{5.1a}$$
$$u_{ttt} \in L^\infty(0,T;L^2(\Omega)), \tag{5.1b}$$
$$w \in H^1(0,T;H^{q+1}(\Omega)). \tag{5.1c}$$

The following estimates hold on Ritz projection

$$\|R_h u\|_{H^1} \leq C\|u\|_{H^1}, \qquad \forall u \in H^1, \tag{5.2a}$$
$$\|u - R_h u\| + h\|u - R_h u\|_{H^1} \leq Ch^{q+1}\|u\|_{H^{q+1}}, \qquad \forall u \in H^{q+1}. \tag{5.2b}$$

For the simplicity, we introduce some notations

$$\delta_\tau \phi^{n+1} =: \frac{\phi^{n+1} - \phi^n}{\tau}, \quad \delta_\tau \phi_h^{n+1} =: \frac{\phi_h^{n+1} - \phi_h^n}{\tau},$$

and the approximation errors

$$\tilde{\xi}_u^{n+1} := u^{n+1} - R_h u^{n+1}, \qquad \hat{\xi}_u^{n+1} := R_h u^{n+1} - u_h^{n+1}, \tag{5.3a}$$
$$\tilde{\xi}_w^{n+1} := w^{n+1} - R_h w^{n+1}, \qquad \hat{\xi}_w^{n+1} := R_h w^{n+1} - w_h^{n+1}, \tag{5.3b}$$
$$\sigma(u^{n+1}) =: u_t^{n+1} - D_\tau R_h u^{n+1}, \qquad \sigma(u^1) =: u_t^1 - \delta_\tau R_h u^1. \tag{5.3c}$$

In our estimates, we first introduce the following Lemma 5.1.

Lemma 5.1. *Suppose that (u,w) is a weak solution to* (2.4a)-(2.4b)*, with the additional regularities. Then for any $\tau, h > 0$, there exists $C > 0$, independent of the τ, h, such that*

$$\|\sigma(u^{n+1})\|^2 \leq C\tau^4 + Ch^{2q+2}, \qquad n \geq 1, \tag{5.4a}$$
$$\|\sigma(u^1)\|^2 \leq C\tau^4 + Ch^{2q+2}, \qquad n = 0. \tag{5.4b}$$

Proof. Using Lemma 2.1 and Ritz projection, we have

$$\begin{aligned}\|\sigma(u^{n+1})\|^2 &= \|u_t^{n+1} - D_\tau u^{n+1} + D_\tau u^{n+1} - D_\tau R_h u^{n+1}\|^2 \\ &= \|R_t^{n+1} + (I-R_h)D_\tau u^{n+1}\|^2 \\ &\leq 2\|R_t^{n+1}\|^2 + 2\|(I-R_h)D_\tau u^{n+1}\|^2 \\ &\leq C\tau^4 + Ch^{2q+2}\|D_\tau u^{n+1}\|^2_{H^{q+1}}. \end{aligned} \tag{5.5}$$

By mean value theorem of integral, we deduce that

$$\begin{aligned}\|D_\tau u^{n+1}\|^2_{H^{q+1}} &= \Big\| \frac{3}{2\tau}(u^{n+1}-u^n) - \frac{1}{2\tau}(u^n - u^{n-1}) \Big\|^2_{H^{q+1}} \\ &= \Big\| \frac{3}{2\tau}\int_{t_n}^{t_{n+1}} u_t dt - \frac{1}{2\tau}\int_{t_{n-1}}^{t_n} u_t dt \Big\|^2_{H^{q+1}} \\ &\leq 2\Big\| \frac{3}{2\tau}\int_{t_n}^{t_{n+1}} u_t dt\Big\|^2_{H^{q+1}} + 2\Big\|\frac{1}{2\tau}\int_{t_{n-1}}^{t_n} u_t dt \Big\|^2_{H^{q+1}} \\ &\leq 2\Big(\frac{3}{2\tau}\int_{t_n}^{t_{n+1}} \|u_t\|_{H^{q+1}} dt\Big)^2 + 2\Big(\frac{1}{2\tau}\int_{t_{n-1}}^{t_n} \|u_t\|_{H^{q+1}} dt \Big)^2 \\ &\leq 2\Big(\frac{3}{2\tau}\int_{t_n}^{t_{n+1}} \|u\|_{W^{1,\infty}(0,T,H^{q+1})} dt\Big)^2 + 2\Big(\frac{1}{2\tau}\int_{t_{n-1}}^{t_n} \|u_t\|_{W^{1,\infty}(0,T,H^{q+1})} dt \Big)^2 \\ &\leq 2\Big(\frac{3}{2\tau}C(t_{n+1}-t_n)\Big)^2 + 2\Big(\frac{1}{2\tau}C(t_n - t_{n-1})\Big)^2 \\ &\leq 2\Big(\frac{3}{2\tau}C\tau\Big)^2 + 2\Big(\frac{1}{2\tau}C\tau\Big)^2 \leq C. \end{aligned} \tag{5.6}$$

Similarly, we can get (5.4b). □

The main result on error estimates for the fully discrete BDF scheme is the following Theorem.

Theorem 5.1. *Assume that* (u^{n+1}, w^{n+1}) *and* (u_h^{n+1}, w_h^{n+1}) *are the solutions of* (2.4a)-(2.4b) *and* (2.11a)-(2.11b)*, respectively. Then, for any* $h,\tau > 0$*, the following key error estimate holds*

$$\sum_{k=0}^{n} \tau \|\nabla \hat{\xi}_w^{k+1}\|^2 + \varepsilon^2 \|\nabla \hat{\xi}_u^{n+1}\|^2 + \sum_{k=0}^{n} 2\beta\tau \|D_\tau \hat{\xi}_u^{k+1}\|^2 \leq C\tau^4 + Ch^{2q}. \tag{5.7}$$

Proof. Subtracting (2.11a)-(2.11b) from (2.4a)-(2.4b) (at $t = t_{n+1}$), we have

$$(\sigma(u^{n+1}), v) + (\nabla \hat{\xi}_w^{n+1}, \nabla v) + (D_\tau \hat{\xi}_u^{n+1}, v) = 0, \tag{5.8a}$$

$$\begin{aligned}&(\hat{\xi}_w^{n+1} + \tilde{\xi}_w^{n+1}, \psi) - (f_1(u^{n+1}) - f_1(u_h^{n+1}), \psi) + (f_2(u^{n+1}) - f_2(u_h^n, u_h^{n-1}), \psi) \\ &\quad - \varepsilon^2(\nabla \hat{\xi}_u^{n+1}, \nabla\psi) - \beta(\sigma(u^{n+1}), \psi) - \beta(D_\tau \hat{\xi}_u^{n+1}, \psi) + A\tau(\nabla(u_h^{n+1} - u_h^n), \nabla \psi_h) = 0. \end{aligned} \tag{5.8b}$$

Setting $v=\hat{\xi}_w^{n+1}$ in (5.8a), $\psi=-D_\tau\hat{\xi}_u^{n+1}$ in (5.8b), respectively, then summing these terms, we arrive at

$$\begin{aligned}&\|\nabla\hat{\xi}_w^{n+1}\|^2+\frac{\varepsilon^2}{4\tau}(\|\nabla\hat{\xi}_u^{n+1}\|^2-\|\nabla\hat{\xi}_u^{n}\|^2+\|\nabla(2\hat{\xi}_u^{n+1}-\hat{\xi}_u^{n})\|^2-\|\nabla(2\hat{\xi}_u^{n}-\hat{\xi}_u^{n-1})\|^2\\&\quad+\|\nabla(\hat{\xi}_u^{n+1}-2\hat{\xi}_u^{n}+\hat{\xi}_u^{n-1})\|^2)+\beta\|D_\tau\hat{\xi}_u^{n+1}\|^2=\sum_{i=1}^{6}M_i,\end{aligned}\tag{5.9}$$

where

$$M_1=-(\sigma(u^{n+1}),\hat{\xi}_w^{n+1}),\qquad M_2=(\tilde{\xi}_w^{n+1},D_\tau\hat{\xi}_u^{n+1}),\tag{5.10a}$$
$$M_3=-(f_1(u^{n+1})-f_1(u_h^{n+1}),D_\tau\hat{\xi}_u^{n+1}),\qquad M_4=(u^{n+1}-2u_h^n+u_h^{n-1},D_\tau\hat{\xi}_u^{n+1}),\tag{5.10b}$$
$$M_5=-\beta(\sigma(u^{n+1}),D_\tau\hat{\xi}_u^{n+1}),\qquad M_6=A\tau(\nabla(u_h^{n+1}-u_h^n),\nabla D_\tau\hat{\xi}_u^{n+1}).\tag{5.10c}$$

By Cauchy-Schwarz inequality and Poincaré inequality and Lemma 5.1, we obtain the following estimates, $\overline{\hat{\xi}_w^{n+1}}$ is the spatial average of $\hat{\xi}_w^{n+1}$

$$\begin{aligned}M_1&\le|(\sigma(u^{n+1}),\hat{\xi}_w^{n+1})|=|(\sigma(u^{n+1}),\hat{\xi}_w^{n+1}-\overline{\hat{\xi}_w^{n+1}})|\\&\le C\|\sigma(u^{n+1})\|\|\nabla\hat{\xi}_w^{n+1}\|\le 4C^2\|\sigma(u^{n+1})\|^2+\frac{1}{16}\|\nabla\hat{\xi}_w^{n+1}\|^2\\&\le C\tau^4+Ch^{2q+2}+\frac{1}{16}\|\nabla\hat{\xi}_w^{n+1}\|^2.\end{aligned}\tag{5.11}$$

Applying Cauchy-Schwarz inequality, Young inequality and the Ritz projection implies that

$$\begin{aligned}M_2&\le|(\tilde{\xi}_w^{n+1},D_\tau\hat{\xi}_u^{n+1})|\le C\|\nabla\tilde{\xi}_w^{n+1}\|\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}\\&\le\frac{16}{\alpha}\|\nabla\tilde{\xi}_w^{n+1}\|^2+\frac{\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2\le Ch^{2q}+\frac{\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2.\end{aligned}\tag{5.12}$$

The following result on M_3 can be obtain

$$\begin{aligned}M_3&\le|(f_1(u^{n+1})-f_1(u_h^{n+1}),D_\tau\hat{\xi}_u^{n+1})|\\&=|(f_1'(\rho)(u^{n+1}-u_h^{n+1}),D_\tau\hat{\xi}_u^{n+1})|\\&\le\|\nabla(u^{n+1}-u_h^{n+1})\|\|f_1'(\rho)D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}\\&\le\frac{16L^2}{\alpha}\|\nabla(u^{n+1}-u_h^{n+1})\|^2+\frac{\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2\\&\le 32L^2Ch^{2q}+32L^2\|\nabla\hat{\xi}_u^{n+1}\|^2+\frac{\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2\\&\le Ch^{2q}+C\|\nabla\hat{\xi}_u^{n+1}\|^2+\frac{\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2.\end{aligned}\tag{5.13}$$

For M_4, we obtain that

$$\begin{aligned}
M_4 =& (u^{n+1}-2u_h^n+u_h^{n-1},D_\tau\hat{\xi}_u^{n+1}) \\
=& (u^{n+1}-2u^n+u^{n-1}+2(u^n-u_h^n)-(u^{n-1}-u_h^{n-1}),D_\tau\hat{\xi}_u^{n+1}) \\
\le& |(u^{n+1}-2u^n+u^{n-1},D_\tau\hat{\xi}_u^{n+1})|+2(u^n-u_h^n,D_\tau\hat{\xi}_u^{n+1})-(u^{n-1}-u_h^{n-1},D_\tau\hat{\xi}_u^{n+1}) \\
\le& \|\nabla(u^{n+1}-2u^n+u^{n-1})\|\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}+2\|\nabla(u^n-u_h^n)\|\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h} \\
&+\|\nabla(u^{n-1}-u_h^{n-1})\|\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h} \\
\le& \frac{16}{\alpha}\|\nabla(u^{n+1}-2u^n+u^{n-1})\|^2+\frac{64}{\alpha}\|\nabla(u^n-u_h^n)\|^2 \\
&+\frac{16}{\alpha}\|\nabla(u^{n-1}-u_h^{n-1})\|^2+\frac{3\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2 \\
\le& C\tau^4+Ch^{2q}+C\|\nabla\hat{\xi}_u^n\|^2+C\|\nabla\hat{\xi}_u^{n-1}\|^2+\frac{3\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2.
\end{aligned} \tag{5.14}$$

By Lemma 5.1 and Young inequality, we get the estimate of M_5

$$\begin{aligned}
M_5 \le& |\beta(\sigma(u^{n+1}),D_\tau\hat{\xi}_u^{n+1})| \le \beta\|\sigma(u^{n+1})\|\|D_\tau\hat{\xi}_u^{n+1}\| \\
\le& \frac{\beta}{2}\|\sigma(u^{n+1})\|^2+\frac{\beta}{2}\|D_\tau\hat{\xi}_u^{n+1}\|^2 \le C\tau^4+Ch^{2q+2}+\frac{\beta}{2}\|D_\tau\hat{\xi}_u^{n+1}\|^2.
\end{aligned} \tag{5.15}$$

For M_6, using Theorem 4.3, we have

$$\begin{aligned}
M_6 =& A\tau(\nabla(u_h^{n+1}-u_h^n),\nabla D_\tau\hat{\xi}_u^{n+1}) \\
=& A\tau(\nabla(u_h^{n+1}-u^{n+1}+u^{n+1}-u^n+u^n-u_h^n),\nabla D_\tau\hat{\xi}_u^{n+1}) \\
=& A\tau(\nabla(\hat{\xi}_u^n-\hat{\xi}_u^{n+1}),\nabla D_\tau\hat{\xi}_u^{n+1})+A\tau(\nabla(u^{n+1}-u^n),\nabla D_\tau\hat{\xi}_u^{n+1}) \\
=& A\tau\Big(\nabla(\hat{\xi}_u^n-\hat{\xi}_u^{n+1}),\nabla\frac{3\hat{\xi}_u^{n+1}-4\hat{\xi}_u^n+\hat{\xi}_u^{n-1}}{2\tau}\Big)+A\tau(\nabla(u^{n+1}-u^n),\nabla D_\tau\hat{\xi}_u^{n+1}) \\
\le& \frac{5A}{4}\|\nabla(\hat{\xi}_u^{n+1}-\hat{\xi}_u^n)\|^2-\frac{A}{4}\|\nabla(\hat{\xi}_u^n-\hat{\xi}_u^{n-1})\|^2+\frac{A}{4}\|\nabla(\hat{\xi}_u^{n+1}-2\hat{\xi}_u^n+\hat{\xi}_u^{n-1})\|^2 \\
&+\frac{16A^2\tau^2}{\alpha}\|\nabla\Delta(u^{n+1}-u^n)\|^2+\frac{\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2 \\
\le& C\|\nabla\hat{\xi}_u^{n+1}\|^2+C\|\nabla\hat{\xi}_u^n\|^2+C\|\nabla\hat{\xi}_u^{n-1}\|^2+C\tau^4+\frac{\alpha}{64}\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2.
\end{aligned} \tag{5.16}$$

Next, we estimate $\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2$. Using Lemma 5.1 and considering that the definition of $\|\cdot\|_{-1,h}$ in (5.8a), we arrive that

$$\begin{aligned}
(D_\tau\hat{\xi}_u^{n+1},v) =& -(\sigma(u^{n+1}),v)-(\nabla\hat{\xi}_w^{n+1},\nabla v) \\
\le& \|\sigma(u^{n+1})\|_{-1,h}\|\nabla v\|+\|\nabla\hat{\xi}_w^{n+1}\|\|\nabla v\| \\
\le& (\|\sigma(u^{n+1})\|_{-1,h}+\|\nabla\hat{\xi}_w^{n+1}\|)\|\nabla v\| \\
\le& (C\tau^2+Ch^{q+1}+\|\nabla\hat{\xi}_w^{n+1}\|)\|\nabla v\|.
\end{aligned} \tag{5.17}$$

Hence

$$\|D_\tau\hat{\xi}_u^{n+1}\|_{-1,h}^2 \le C\tau^4 + Ch^{2q+2} + 3\|\nabla\hat{\xi}_w^{n+1}\|^2. \tag{5.18}$$

Taking α properly, substituting M_1-M_6 into (5.9), and multiplying by 4τ, lead to the following result

$$\begin{aligned}&\tau\|\nabla\hat{\xi}_w^{n+1}\|^2 + (\|\nabla\hat{\xi}_u^{n+1}\|^2 - \|\nabla\hat{\xi}_u^n\|^2 + \|\nabla(2\hat{\xi}_u^{n+1} - \hat{\xi}_u^n)\|^2 - \|\nabla(2\hat{\xi}_u^n - \hat{\xi}_u^{n-1})\|^2 \\ &\quad + \|\nabla(\hat{\xi}_u^{n+1} - 2\hat{\xi}_u^n + \hat{\xi}_u^{n-1})\|^2) + 2\beta\tau\|D_\tau\hat{\xi}_u^{n+1}\|^2 \\ &\le C\tau\tau^4 + C\tau h^{2q} + C\tau\|\nabla\hat{\xi}_u^{n+1}\|^2 + C\tau\|\nabla\hat{\xi}_u^n\|^2 + C\tau\|\nabla\hat{\xi}_u^{n-1}\|^2. \end{aligned} \tag{5.19}$$

Summing the above inequalities over $k=1,\cdots n$ and using Gronwall inequality, we get

$$\begin{aligned}&\sum_{k=1}^n \tau\|\nabla\hat{\xi}_w^{k+1}\|^2 + \varepsilon^2\|\nabla\hat{\xi}_u^{n+1}\|^2 + \sum_{k=1}^n 2\beta\tau\|D_\tau\hat{\xi}_u^{k+1}\|^2 \\ &\le \|\nabla\hat{\xi}_u^1\|^2 + \|\nabla(2\hat{\xi}_u^1 - \hat{\xi}_u^0)\|^2 + CT\tau^4 + CTh^{2q}. \end{aligned} \tag{5.20}$$

Next, we subtract (2.13a)-(2.13b) from (2.4a)-(2.4b) (at $t=t_1$) to estimate $\|\nabla\hat{\xi}_u^1\|^2$,

$$(\sigma(u^1),v) + (\nabla\hat{\xi}_w^1,\nabla v) + (\delta_\tau\hat{\xi}_u^1,v) = 0, \tag{5.21a}$$

$$\begin{aligned}&(\hat{\xi}_w^1 + \tilde{\xi}_w^1,\psi) - (f_1(u^1) - f_2(u^1),\psi) + (f_1(u_h^1) - f_2(u_h^0),\psi) \\ &\quad - \varepsilon^2(\nabla\hat{\xi}_u^1,\nabla\psi) - \beta(\sigma(u^1),\psi) - \beta(\delta_\tau\hat{\xi}_u^1,\psi) = 0. \end{aligned} \tag{5.21b}$$

Setting $v=\hat{\xi}_w^1$ in (5.21a), $\psi=-\delta_\tau\hat{\xi}_u^1$ in (5.21b), respectively, multiplying τ, then summing these terms, we have

$$\tau\|\nabla\hat{\xi}_w^1\|^2 + \frac{\varepsilon^2}{2}(\|\nabla\hat{\xi}_u^1\|^2 - \|\nabla\hat{\xi}_u^0\|^2 + \|\nabla\hat{\xi}_u^1 - \nabla\hat{\xi}_u^0\|^2) + \beta\tau\|\delta_\tau\hat{\xi}_u^1\|^2 = \sum_{i=1}^5 \tau J_i, \tag{5.22}$$

where

$$J_1 = -(\sigma(u^1),\hat{\xi}_w^1), \qquad J_2 = (\tilde{\xi}_w^1,\delta_\tau\hat{\xi}_u^1), \tag{5.23a}$$

$$J_3 = -(f_1(u^1) - f_1(u_h^1),\delta_\tau\hat{\xi}_u^1), \qquad J_4 = (u^1 - u_h^0,\delta_\tau\hat{\xi}_u^1), \tag{5.23b}$$

$$J_5 = -\beta(\sigma(u^1),\delta_\tau\hat{\xi}_u^1). \tag{5.23c}$$

Similar to previous analysis, we can obtain the following estimates

$$\tau J_1 = -\tau(\sigma(u^1),\hat{\xi}_w^1) \le C\tau^2\|\sigma(u^1)\|_{-1,h}^2 + \frac{\alpha}{5}\|\nabla\hat{\xi}_w^1\|^2 \le C\tau^4 + \frac{\alpha}{5}\|\nabla\hat{\xi}_w^1\|^2, \tag{5.24a}$$

$$\tau J_2 = \tau(\tilde{\xi}_w^1,\delta_\tau\hat{\xi}_u^1) \le \frac{C\tau^2}{\alpha}\|\nabla\tilde{\xi}_w^1\|^2 + \frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2 \le C\tau^2h^{2q} + \frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2, \tag{5.24b}$$

$$\begin{aligned}\tau J_3 &= -\tau(f_1(u^1) - f_1(u_h^1),\delta_\tau\hat{\xi}_u^1) \le \frac{C\tau^2L^2}{\alpha}\|\nabla(u^1 - u_h^1)\|^2 + \frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2 \\ &\le C\tau^2h^{2q} + C\tau^2\|\nabla\hat{\xi}_u^1\|^2 + \frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2, \end{aligned} \tag{5.24c}$$

$$\tau J_4=\tau(u^1-u_h^0,\delta_\tau\hat{\xi}_u^1)\leq\frac{C\tau^2}{\alpha}\|\nabla(u^1-u^0+u^0-u_h^0)\|^2+\frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2$$
$$\leq C\tau^4+C\tau^2h^{2q}+C\tau^2\|\nabla\hat{\xi}_u^0\|^2+\frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2, \tag{5.24d}$$
$$\tau J_5=-\beta\tau(\sigma(u^1),\delta_\tau\hat{\xi}_u^1)\leq\frac{C\tau^2\beta^2}{\alpha}\|\sigma(u^1)\|^2+\frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2\leq C\tau^4+\frac{\alpha}{15}\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2. \tag{5.24e}$$

As well as the similar analysis applied to (5.17), one gets

$$\|\delta_\tau\hat{\xi}_u^1\|_{-1,h}^2\leq C\tau^4+Ch^{2q+2}+3\|\nabla\hat{\xi}_w^1\|^2. \tag{5.25}$$

Considering that (5.24a)-(5.25), we arrive at

$$\tau\|\nabla\hat{\xi}_w^1\|^2+\varepsilon^2\|\nabla\hat{\xi}_u^1\|^2+2\beta\tau\|\delta_\tau\hat{\xi}_u^1\|^2\leq C\tau^4+Ch^{2q}+\alpha\|\nabla\hat{\xi}_w^1\|^2. \tag{5.26}$$

Taking α properly

$$\tau\|\nabla\hat{\xi}_w^1\|^2+\varepsilon^2\|\nabla\hat{\xi}_u^1\|^2+\beta\tau\|\delta_\tau\hat{\xi}_u^1\|^2\leq C\tau^4+Ch^{2q}. \tag{5.27}$$

Combining (5.20) and (5.27) yields the following result

$$\sum_{k=0}^{n}\tau\|\nabla\hat{\xi}_w^{k+1}\|^2+\varepsilon^2\|\nabla\hat{\xi}_u^{n+1}\|^2+\sum_{k=0}^{n}2\beta\tau\|D_\tau\hat{\xi}_u^{k+1}\|^2\leq C\tau^4+Ch^{2q}. \tag{5.28}$$

Thus, we complete the proof. □

6 Numerical experiments

In this section, we apply the fully discrete second order BDF scheme to perform a numerical accuracy check. In the following simulation, for u and w, we take the P2 finite element space, the parameter $q=2$. The nonlinear equation is solved by the classical Newton's method. All tests are performed by the Freefem++ package [60].

6.1 Convergence and energy dissipation

In this part, we perform verification and validation of the theoretical error estimates and stability analysis by numerical examples, i.e., verification of the order of convergence and dissipation of energy of our scheme for the viscous Cahn-Hilliard equation. The viscous Cahn-Hilliard equation is defined in the domain $[0,1]\times[0,1]$ with the initial condition

$$u_0=0.24\cos(2\pi x)\cos(2\pi y)+0.4\cos(\pi x)\cos(3\pi y).$$

Tables 1-3 list the spatial convergence order of u with Flory-Huggins potential. The parameters are chosen as follows: ε=0.09,0.1,0.2, θ=0.7, k=0.1, β=0.01, τ=0.01, T=0.02,

Table 1: The spatial convergence rate of $\hat{\xi}_u$ with $\varepsilon=0.09$.

$A=\frac{1}{16}$	h	$\frac{h}{2}$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate	$A=1$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate
	$\frac{3.2}{32}$	$\frac{3.2}{64}$	0.0637182			0.0682649	
	$\frac{3.2}{64}$	$\frac{3.2}{128}$	0.0143694	2.1487		0.0154592	2.14268
	$\frac{3.2}{128}$	$\frac{3.2}{256}$	0.00339356	2.08213		0.00365134	2.08197
	$\frac{3.2}{256}$	$\frac{3.2}{512}$	0.00080422	2.07714		0.000864693	2.07817

Table 2: The spatial convergence rate of $\hat{\xi}_u$ with $\varepsilon=0.1$.

$A=\frac{1}{16}$	h	$\frac{h}{2}$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate	$A=1$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate
	$\frac{3.2}{32}$	$\frac{3.2}{64}$	0.0544225			0.0593425	
	$\frac{3.2}{64}$	$\frac{3.2}{128}$	0.012259	2.15036		0.0134308	2.14351
	$\frac{3.2}{128}$	$\frac{3.2}{256}$	0.00289257	2.08341		0.00317119	2.08246
	$\frac{3.2}{256}$	$\frac{3.2}{512}$	0.000685304	2.07754		0.000751013	2.07811

Table 3: The spatial convergence rate of $\hat{\xi}_u$ with $\varepsilon=0.2$.

$A=\frac{1}{16}$	h	$\frac{h}{2}$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate	$A=1$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate
	$\frac{3.2}{32}$	$\frac{3.2}{64}$	0.00506491			0.00734155	
	$\frac{3.2}{64}$	$\frac{3.2}{128}$	0.00116066	2.12559		0.0017038	2.10733
	$\frac{3.2}{128}$	$\frac{3.2}{256}$	0.000260445	2.15589		0.000393238	2.11528
	$\frac{3.2}{256}$	$\frac{3.2}{512}$	$5.90964e-005$	2.13984		$9.14572e-005$	2.10423

Table 4: The spatial convergence rate of $\hat{\xi}_u$.

$\beta=0$	h	$\frac{h}{2}$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate	$\beta=0.0001$	$\Vert\hat{\xi}_u\Vert_{H^1}$	rate
	$\frac{3.2}{32}$	$\frac{3.2}{64}$	0.0385997			0.0388075	
	$\frac{3.2}{64}$	$\frac{3.2}{128}$	0.0090509	2.09246		0.00909236	2.09361
	$\frac{3.2}{128}$	$\frac{3.2}{256}$	0.00210044	2.10737		0.00211191	2.10611
	$\frac{3.2}{256}$	$\frac{3.2}{512}$	0.000490416	2.09861		0.000493424	2.09765

$h=\frac{3.2}{32}, \frac{3.2}{64}, \frac{3.2}{128}, \frac{3.2}{256}$. The spatial convergence orders computed from the error $\Vert\hat{\xi}_u\Vert_{H^1}$ are close to 2.

Tables 4-6 list the spatial convergence order of u with variable β. The parameters are chosen as follows : $\beta=0,0.0001,0.001,0.01,0.1,1$, $\varepsilon=0.1$, $\theta=0.7$, $k=0.1$, $\beta=0.01$, $\tau=0.01$, $T=0.02$, $h=\frac{3.2}{32},\frac{3.2}{64},\frac{3.2}{128},\frac{3.2}{256}$. The spatial convergence orders computed from the error $\Vert\hat{\xi}_u\Vert_{H^1}$ are close to 2.

6.1.1 the order of convergence in time

Table 7 and Table 8 show the time convergence order of u with variable A. We choose parameters as follows: $\varepsilon=0.1$, $\theta=0.0007$, $\beta=0.2$, $h=\tau=0.125,0.0625,0.03125$, $T=0.2$. The time convergence orders computed from errors $\Vert\hat{\xi}_u\Vert_{H^1}$ are close to 2. These numerical results imply that our numerical algorithm is correct.

Table 5: The spatial convergence rate of $\hat{\xi}_u$.

$\beta=0.001$	h	$\frac{h}{2}$	$\|\hat{\xi}_u\|_{H^1}$	rate	$\beta=0.01$	$\|\hat{\xi}_u\|_{H^1}$	rate
	$\frac{3.2}{32}$	$\frac{3.2}{64}$	0.0407566			0.0593425	
	$\frac{3.2}{64}$	$\frac{3.2}{128}$	0.00948613	2.10314		0.0134308	2.14351
	$\frac{3.2}{128}$	$\frac{3.2}{256}$	0.0022176	2.09682		0.00317119	2.08246
	$\frac{3.2}{256}$	$\frac{3.2}{512}$	0.000520659	2.09059		0.000751013	2.07811

Table 6: The spatial convergence rate of $\hat{\xi}_u$.

$\beta=0.1$	h	$\frac{h}{2}$	$\|\hat{\xi}_u\|_{H^1}$	rate	$\beta=1$	$\|\hat{\xi}_u\|_{H^1}$	rate
	$\frac{3.2}{32}$	$\frac{3.2}{64}$	0.103198			0.118354	
	$\frac{3.2}{64}$	$\frac{3.2}{128}$	0.0231641	2.15545		0.0265937	2.15395
	$\frac{3.2}{128}$	$\frac{3.2}{256}$	0.00538281	2.10546		0.00615805	2.11054
	$\frac{3.2}{256}$	$\frac{3.2}{512}$	0.00126241	2.09218		0.00143901	2.0974

Table 7: The temporal convergence rate of $\hat{\xi}_u$.

$A=0$	τ	$\|\hat{\xi}_u\|_{H^1}$	rate	$A=\frac{1}{16}$	$\|\hat{\xi}_u\|_{H^1}$	rate
	0.125	0.813833			0.815218	
	0.0625	0.212451	1.9376		0.21013	1.9559
	0.03125	0.055102	1.94695		0.0521946	2.00931

Table 8: The temporal convergence rate of $\hat{\xi}_u$.

$A=1$	τ	$\|\hat{\xi}_u\|_{H^1}$	rate	$A=2$	$\|\hat{\xi}_u\|_{H^1}$	rate
	0.125	0.821489			0.823136	
	0.0625	0.20555	1.99875		0.204805	2.00688
	0.03125	0.047327	2.11875		0.0492607	2.05574

6.1.2 Energy dissipation

Now, let us verify the energy dissipation of our proposed scheme. The energy function of the viscous Cahn-Hilliard equation is

$$E(u_h^{n+1})=\int_\Omega\Big(\frac{\varepsilon^2}{2}|\nabla u_h^{n+1}|^2+F(u_h^{n+1})\Big)dx,$$

and the modified energy function of the fully discrete scheme is defined as

$$\Xi(u_h^{n+1},u_h^n)=:E(u_h^{n+1})+\frac{1}{4\tau}\|u_h^{n+1}-u_h^n\|_{-1,h}^2+\frac{1}{2}\|u_h^{n+1}-u_h^n\|^2+\frac{\beta}{4\tau}\|u_h^{n+1}-u_h^n\|^2.$$

We can see that energy function is non-increasing in Fig. 1 with different value of A. Indeed, the numerical energy stability can be observed for any $A\geq 0$. Here the parameters are $\theta=0.7$, $k=0.01$, $\varepsilon=0.1$, $h=\frac{1}{32}$, $\tau=0.01$, $T=0.1$.

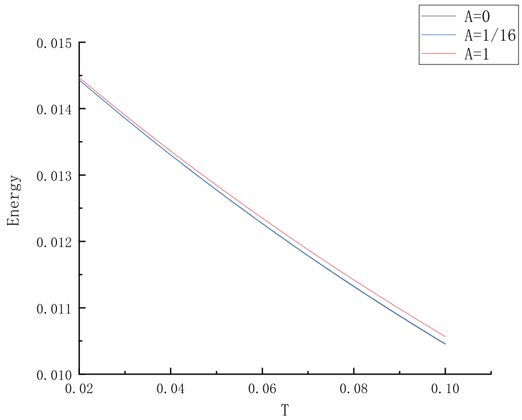

Figure 1: The evolutions of discrete energy.

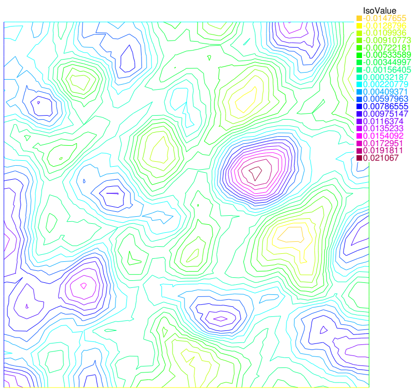

Figure 2: $T=0.0001$s.

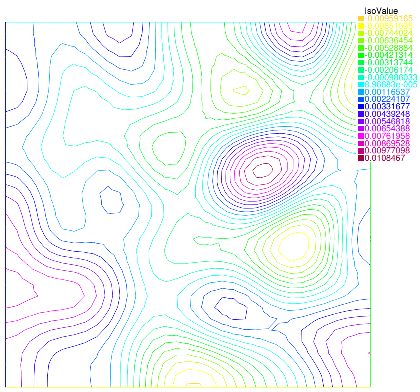

Figure 3: $T=0.0005$s.

6.2 Spinodal decomposition

In this test, we simulate the process of spinodal decomposition (phase separation behavior) on viscous Cahn-Hilliard equation with logarithmic Flory-Huggins potential (Figs. 2-9). The process of the phase separation can be studied in a binary mixture, which is quenched into the unstable part of its miscibility gap. In this case, the spinodal decomposition takes place, which reflected in the natural growth of the concentration variations that makes the system from the homogeneous to the two-phase state.

The simulation is done in the domain $[0,1]\times[0,1]$ with the parameters $\tau=0.0001$, $\theta=0.5$, $\varepsilon=0.2$. The initial condition is taken as a random field value

$$u_0=0.01*rand()-0.05,$$

where rand$\in[0,1]$.

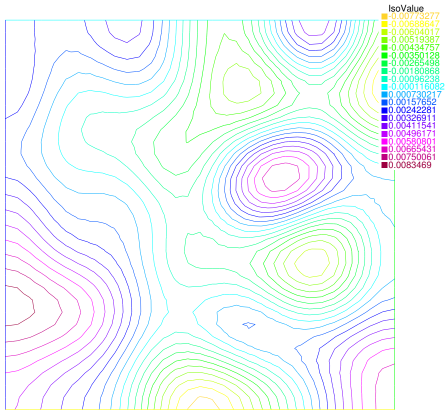

Figure 4: $T=0.001$s.

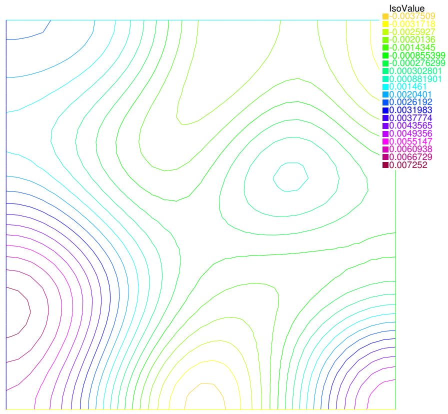

Figure 5: $T=0.005$s.

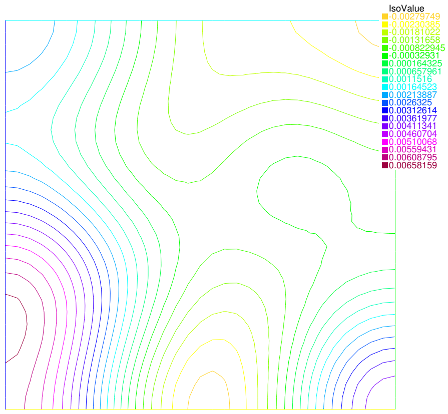

Figure 6: $T=0.01$s.

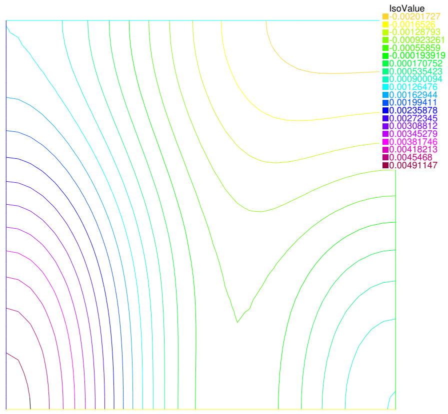

Figure 7: $T=0.05$s.

7 Conclusions

In this paper we have developed a second order BDF-type scheme for the viscous Cahn-Hilliard equation with logarithmic Flory-Huggins potential that is unconditionally stable in energy. The convergence rates are shown to be $o(h^2)$ in H^1-norm of u. The theoretical results are verifiered by numerical experiments which also indicate that our proposed method is effective.

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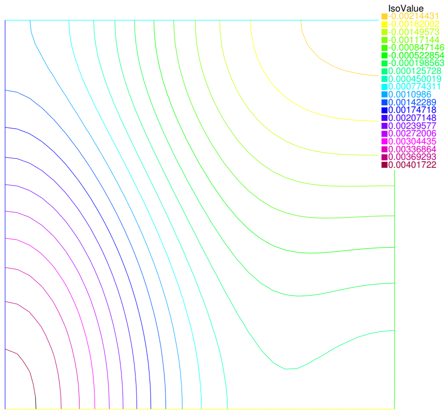

Figure 8: $T = 0.1$s.

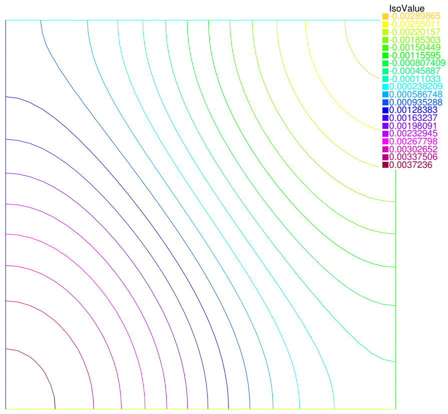

Figure 9: $T = 0.5$s.

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