

A New Multi-Step BDF Energy Stable Technique for the Extended Fisher–Kolmogorov Equation

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Abstract. The multi-step backward difference formulas of order k (BDF- k) for $3 \leq k \leq 5$ are proposed for solving the extended Fisher–Kolmogorov equation. Based upon the careful discrete gradient structures of the BDF- k formulas, the suggested numerical schemes are proved to preserve the energy dissipation laws at the discrete levels. The maximum norm priori estimate of the numerical solution is established by means of the energy stable property. With the help of discrete orthogonal convolution kernels techniques, the L^2 norm error estimates of the implicit BDF- k schemes are established. Several numerical experiments are included to illustrate our theoretical results.

Keywords: extended Fisher-Kolmogorov equation, multi-step BDF method, discrete orthogonal convolution kernels, stability and convergence.

AMS Subject Classification: 65M06; 65M12.

1 Introduction

In this paper, we are interested in developing the rigorous stability and convergence analysis of BDF-k ($k = 3, 4, 5$) for simulating the extended Fisher-Kolmogorov (EFK) model [3, 9, 10].

$$\begin{aligned} \partial_t \Phi &= \Delta \Phi - \gamma \Delta^2 \Phi - f(\Phi) \quad \text{for } \mathbf{x} \in \Omega \text{ and } 0 < t \leq T, \\ \Phi(\cdot, t) &\text{ is } L\text{-periodic, } t \in (0, T), \\ \Phi(\mathbf{x}, 0) &:= \Phi_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \end{aligned} \tag{1.1}$$

where the spatial domain $\Omega = (0, L)^2 \subset \mathbb{R}^2$, the nonlinear function $f(v) = v^3 - v$, the parameter $\gamma > 0$ is a positive constant and $\Phi_0(\mathbf{x})$ is a given L -periodic function regular enough. Mathematically, the governing system of the EFK model could be derived via an L^2 gradient flow associated with the the following free energy (Lyapunov) functional

$$E[\Phi] = \int_{\Omega} \left(\frac{\gamma}{2} |\Delta \Phi|^2 + \frac{1}{2} |\nabla \Phi|^2 + F[\Phi] \right) dx.$$

Then, the system has the energy dissipation law

$$\frac{dE}{dt} = \left(\frac{\delta E}{\delta \Phi}, \partial_t \Phi \right) = - \|\partial_t \Phi\|_{L^2}^2 \leq 0,$$

in which $(f, g) := \int_{\Omega} fg \, d\mathbf{x}$, and the associated L^2 norm $\|f\|_{L^2} = \sqrt{(f, f)}$ for all $f, g \in L^2(\Omega)$.

The EFK model was proposed by adding a fourth order derivative term to the classical Fisher-Kolmogorov (FK) model by Couillet, Elphick and Repauxin in [4]. Then the generalization of the standard FK model was explored by Dee and Saarloos in [6]. The EFK model has wide applications in science and technology. The numerical methods, including finite element Galerkin method [5, 8], collocation method [25] and pseudo-spectral method [16] for solving the EFK model had attracted many researchers. The numerical research in [11, 12, 13, 14, 15] are mainly focused on the Crank-Nicolson (CN) type schemes with uniform time-step. However, it is well known that the BDF method is a class of implicit methods for solving rigid differential equation numerical integrals. They are linear multistep methods, which use the information of the time point to approximate the derivative of the unknown function, thus improving the approximation accuracy. These methods are particularly suitable for the solution of rigid differential equation in which the numerical stability is expressed as an absolutely stable region which it is called A-stable. It is well known that only the first-order and second-order backward differential formulas (BDF1 and BDF2) are A-stable, see [27], while orders greater than 2 can not be A-stable. Some remedial measures [1, 2, 24] have been proposed to restore the the L^2 norm stability and convergence for k-order backward differential formula ($k = 3, 4, 5$). It is worthwhile to noting that this standard analysis technique of BDF-k methods may not be used to establish some discrete energy stable property for the gradient flow systems, including the EFK equation.

In this paper, we will make use of the recent discrete orthogonal convolution (DOC) technique to analyze the BDF-k time-stepping method for solving the EFK equation. The readers are referred to [17, 19, 20, 23] for the adaptive BDF2 methods for the convergence analysis of linear reaction-diffusion problem and the phase field models. Consider the time-step sizes $\tau := T/N$ and the uniform discrete time layers $t_j = j\tau$. For any grid function $\{v^k\}_{k=0}^N$, put $\nabla_\tau v^n := v^n - v^{n-1}$ and $\partial_\tau v^n := \nabla_\tau v^n / \tau$. When the index $k = 3, 4$ or 5 , the BDF-k formula $D_k v^n$ with uniform time-steps reads

$$D_k v^n := \frac{1}{\tau} \sum_{k=1}^n b_{n-k}^{(k)} \nabla_\tau v^k, \quad n \geq k,$$

where the associated BDF-k kernels $b_j^{(k)}$ (vanish if $j \geq k$), see Table 1, are generated by

$$\sum_{\ell=1}^k \frac{1}{\ell} (1 - \zeta)^{\ell-1} = \sum_{\ell=0}^{k-1} b_\ell^{(k)} \zeta^\ell, \quad 3 \leq k \leq 5. \tag{1.2}$$

Table 1. The BDF-k kernels $b_j^{(k)}$ generated by (1.2).

BDF-k	$b_0^{(k)}$	$b_1^{(k)}$	$b_2^{(k)}$	$b_3^{(k)}$	$b_4^{(k)}$
k = 2	$\frac{3}{2}$	$-\frac{1}{2}$			
k = 3	$\frac{11}{6}$	$-\frac{7}{6}$	$\frac{1}{3}$		
k = 4	$\frac{25}{12}$	$-\frac{23}{12}$	$\frac{13}{12}$	$-\frac{1}{4}$	
k = 5	$\frac{137}{60}$	$-\frac{163}{60}$	$\frac{137}{60}$	$-\frac{21}{20}$	$\frac{1}{5}$

In order to analyze the L^2 norm stability and convergence of the BDF-k methods, the corresponding DOC kernels technique will be introduced. For the discrete BDF-k kernels $b_j^{(k)}$ generated by (1.2), the corresponding DOC-k kernels $\theta_j^{(k)}$ are defined by [22]

$$\theta_0^{(k)} := \frac{1}{b_0^{(k)}}, \quad \theta_{n-j}^{(k)} := -\frac{1}{b_0^{(k)}} \sum_{\ell=j+1}^n \theta_{n-\ell}^{(k)} b_{\ell-j}^{(k)}, \quad j=n-1, n-2, \dots, k+1, k. \tag{1.3}$$

According to the above expressions, we can find the following discrete orthogonal convolution property

$$\sum_{\ell=j}^n \theta_{n-\ell}^{(k)} b_{\ell-j}^{(k)} \equiv \delta_{nj} \quad \text{for any } k \leq j \leq n, \tag{1.4}$$

where δ_{nk} is the Kronecker delta symbol. Thus, this characteristic leads directly to the following relationship, yields

$$\sum_{j=k}^n \theta_{n-j}^{(k)} \sum_{\ell=k}^j b_{j-\ell}^{(k)} \nabla_\tau \phi^\ell = \sum_{\ell=k}^n \nabla_\tau \phi^\ell \sum_{j=\ell}^n \theta_{n-j}^{(k)} b_{j-\ell}^{(k)} = \nabla_\tau \phi^n \quad \text{for } k \leq n \leq N.$$

This identity directly leads to the following relationship

$$\begin{aligned} \sum_{j=k}^n \theta_{n-j}^{(k)} D_k \phi^j &= \frac{1}{\tau} \sum_{j=k}^n \theta_{n-j}^{(k)} \sum_{\ell=1}^{k-1} b_{j-\ell}^{(k)} \nabla_{\tau} \phi^{\ell} + \frac{1}{\tau} \sum_{j=k}^n \theta_{n-j}^{(k)} \sum_{\ell=k}^j b_{j-\ell}^{(k)} \nabla_{\tau} \phi^{\ell} \\ &\triangleq \frac{1}{\tau} \phi_1^{(k,n)} + \partial_{\tau} \phi^n \quad \text{for } k \leq n \leq N, \end{aligned} \quad (1.5)$$

which $\phi_1^{(k,n)}$ is defined as

$$\phi_1^{(k,n)} := \sum_{\ell=1}^{k-1} \nabla_{\tau} \phi^{\ell} \sum_{j=k}^n \theta_{n-j}^{(k)} b_{j-\ell}^{(k)} \quad \text{for } n \geq k. \quad (1.6)$$

With the aid of the discrete convolution kernels, we focus on the effectiveness of numerical method by considering a fully implicit BDF- k approach for solving the EFK equation (1.1). Denote the space of L -periodic grid functions $\mathbb{V}_h := \{v_h \mid v_h \text{ is } L\text{-periodic for } \mathbf{x}_h \in \bar{\Omega}_h\}$. That is, to find the numerical solution $\phi_h^n \in \mathbb{V}_h$ such that

$$D_k \phi_h^n + \gamma \Delta_h^2 \phi_h^n + f(\phi_h^n) - \Delta_h \phi_h^n = 0 \quad \text{for } \mathbf{x}_h \in \Omega_h \text{ and } k \leq n \leq N, \quad (1.7)$$

subjected to the initial value $\phi_h^0 = \Phi_0(\mathbf{x}_h)$ and periodic boundary conditions. Always, to avoid complex theoretical analysis, it is to assume that the initial solutions ϕ_h^{ℓ} for $1 \leq \ell \leq k-1$ have been obtained by choose other higher-order numerical algorithms, such as the Runge-Kutta method. The equivalent convolutional form of the scheme (1.7) using DOC kernel technology will play an important role in our analysis.

By applying the DOC- k kernels $\theta_{j-n}^{(k)}$ to both sides of the discrete formula (1.7) with the help of (1.5) and (1.6), one can obtain the following equivalent schemes (replacing n by ℓ)

$$\partial_{\tau} \phi^j = -\phi_1^{(k,j)} / \tau + \sum_{\ell=k}^j \theta_{j-\ell}^{(k)} (\Delta_h \phi_h^{\ell} - \gamma \Delta_h^2 \phi_h^{\ell} - f(\phi_h^{\ell})) \quad \text{for } j \geq k. \quad (1.8)$$

In this article, we emphasize that the convolution formula will be the core and starting point of our energy technology, potentially producing a simpler and more effective proof than previous work [1, 2, 24]. Our work is organized as follows. The unique solvability of the fully implicit BDF- k scheme (1.7) is established, see Theorem 1. Then, the energy dissipation law in Theorem 2 is verified and Theorem 3 can establish the boundedness of solution in the maximum norm in Section 2. In Section 3, an optimal L^2 norm error estimate of the BDF- k scheme (1.7) is established with the help of the DOC kernels. It is worthy mentioning that, this is the first time to extend the stability and convergence theory of the BDF- k scheme for solving the EFK equation. Several numerical experiments are presented in Section 4 to show the accuracy and effectiveness of our BDF- k method.

2 Solvability and energy dissipation law

2.1 Spatial dispersion

For a completed presentation of the discrete numerical scheme, we describe the general situation of spatial discretization briefly.

For the domain $\Omega = (0, L)^2$, let the grid length $h_x = h_y = h := L/M$ with an integer M . Let put the full discrete spatial grid $\bar{\Omega}_h := \{x_h = (ih, jh) \mid 0 \leq i, j \leq M\}$ and define $\Omega_h := \{x_h = (ih, jh) \mid 1 \leq i, j \leq M\}$. For the function $v_h = v(x_h)$, let $\Delta_x v_{ij} := (v_{i+1,j} - v_{i,j})/h$ and $\delta_x^2 v_{ij} = (v_{i+1,j} - 2v_{i,j} + v_{i-1,j})/h^2$. Similarly, $\Delta_y v_{ij}$ and $\delta_y^2 v_{ij}$ can be defined. Then the discrete Laplacian and gradient vector are $\Delta_h v_{ij} := (\delta_x^2 + \delta_y^2)v_{ij}$ and $\nabla_h v_{ij} := (\Delta_x v_{ij}, \Delta_y v_{ij})^T$ respectively. For any $v, w \in \mathbb{V}_h$, we define the discrete inner products and norms as follows:

$$\langle v, w \rangle := h^2 \sum_{x_h \in \Omega_h} v_h w_h, \quad \|v\| := \sqrt{\langle v, v \rangle}, \quad \|\nabla_h v\| := \left(h^2 \sum_{x_h \in \Omega_h} |\nabla_h v_h|^2 \right)^{\frac{1}{2}},$$

$$\|\Delta_h v\| := \left(h^2 \sum_{x_h \in \Omega_h} |\Delta_h v_h|^2 \right)^{\frac{1}{2}}, \quad \|v\|_\infty := \max_{x_h \in \Omega_h} |v_h|.$$

There exists a positive constant c_Ω which depends on the spatial domain Ω_h , one has the Sobolev inequality in [29]

$$\|v\|_\infty \leq c_\Omega (\|v\| + \|\Delta_h v\|) \quad \text{for } v \in \mathbb{V}_h.$$

Under periodic boundary conditions, for any $v, w \in \mathbb{V}_h$, the discrete Green's formula is shown

$$\langle \Delta_h^2 v, w \rangle = \langle \Delta_h v, \Delta_h w \rangle \quad \text{and} \quad \langle -\Delta_h v, w \rangle = \langle \nabla_h v, \nabla_h w \rangle.$$

2.2 Unique solvability

The following proof shows that the solvability of the implicit BDF-k scheme (1.7) is equivalent to the minimization of a convex functional S according to [28], and also shows that the implicit scheme is uniquely solvable.

Theorem 1. *If the time-step size satisfy the restriction $\tau \leq b_0^{(k)}$, the implicit BDF-k scheme (1.7) is uniquely solvable.*

Proof. For any time-level index $n \geq k$, consider the following discrete energy convex functional S on the space \mathbb{V}_h ,

$$S[\beta] := \frac{1}{2\tau} \langle b_0^{(k)} (\beta - \phi^{n-1}) + 2Q^{n-1}, \beta - \phi^{n-1} \rangle + \frac{\gamma}{2} \|\Delta_h \beta\|^2 + \frac{1}{2} \|\nabla_h \beta\|^2 + \frac{1}{4} \langle (1 - \beta^2)^2, 1 \rangle,$$

where $Q^{n-1} := \sum_{\ell=1}^{n-1} b_{n-\ell}^{(k)} \nabla_\tau \phi^\ell$. Under the time-step condition $\tau \leq b_0^{(k)}$, S is strictly convex function for any $\lambda \in \mathbb{R}$ and any $\psi_h \in \mathbb{V}_h$, due to

$$\frac{d^2 S}{d\lambda^2} [\beta + \lambda\psi] \Big|_{\lambda=0} = \left(\frac{1}{\tau} b_0^{(k)} - 1 \right) \|\psi\|^2 + \gamma \|\Delta_h \psi\|^2 + \|\nabla_h \psi\|^2 + 3\|\beta\psi\|^2 \geq 0.$$

The above result shows that the functional S has a unique minimizing value, denoted by ϕ_h^n , if and only if it solves the equation

$$\begin{aligned} \frac{dS}{d\lambda} [\beta + \lambda\psi] \Big|_{\lambda=0} &= \frac{1}{\tau} \langle b_0^{(k)} (\beta - \phi^{n-1}) + Q^{n-1}, \psi \rangle + \gamma \langle \Delta_h \beta, \Delta_h \psi \rangle + \langle \nabla_h \beta, \nabla_h \psi \rangle \\ &+ \langle f(\beta), \psi \rangle = \frac{1}{\tau} \langle b_0^{(k)} (\beta - \phi^{n-1}) + Q^{n-1} + \gamma \Delta_h^2 \beta - \Delta_h \beta + \beta^3 - \beta, \psi \rangle. \end{aligned}$$

Therefore, for any $\psi_h \in \mathbb{V}_h$, the following equation is obtained, only when we take the unique minimum value $\phi_h^n \in \mathbb{V}_h$,

$$\frac{1}{\tau} \sum_{\ell=1}^n b_{n-\ell}^{(k)} \nabla_\tau \phi^\ell + \gamma \Delta_h^2 \phi^n - \Delta_h \phi^n + (\phi^n)^3 - \phi^n = 0,$$

which is precisely our BDF-k implicit formula (1.7) we constructed. \square

2.3 Energy dissipation property

In what follows, we prove that the numerical scheme (1.7) maintains the modified energy dissipation property at the discrete levels.

Lemma 1. [22, Lemma 2.4] *With the aid of the Grenander-Szegö theorem, see this article [7, pp. 64–65], for $3 \leq k \leq 5$, the discrete BDF-k kernels $b_j^{(k)}$ defined in (1.2) are positive definite in the sense that*

$$2 \sum_{\ell=k}^n w_\ell \sum_{j=k}^{\ell} b_{\ell-j}^{(k)} w_j \geq m_{1k} \sum_{\ell=k}^n w_\ell^2 \quad \text{for } n \geq k,$$

which the constants are $m_{13} = 95/48$, $m_{14} = 1.628$ and $m_{15} = 0.4776$.

Lemma 2. [18, Lemma 2.3] *For any real sequence $\{v_k \mid k = 0, 1, 2, \dots, N\}$, the difference operators are defined when $m \geq 1$ as*

$$\delta_1^{m+1} v_n := \delta_1^m (\delta_1 v_n) = \delta_1^m v_n - \delta_1^m v_{n-1},$$

also define the operator $\delta_1 v_n := \delta_1^1 v_n = v_n - v_{n-1}$. Then for $k = 3, 4$ and 5 , the BDF-k kernels $b_j^{(k)}$ can meet the following form:

$$v_n \sum_{j=1}^n b_{n-j}^{(k)} v_j = \mathcal{G}_k[v_n] - \mathcal{G}_k[v_{n-1}] + \frac{\sigma_{Lk}}{2} v_n^2 + \mathcal{R}_k[v_n] \quad \text{for } n \geq k,$$

where the functionals \mathcal{G}_k , \mathcal{R}_k , and the positive constants σ_{Lk} are shown by

- for $k = 3$, the constant $\sigma_{L3} := \frac{95}{48} \approx 1.979$,

$$\mathcal{G}_3[v_n] := \frac{37}{96} v_n^2 - \frac{1}{8} v_{n-1}^2 + \frac{7}{24} (\delta_1 v_n)^2 = \frac{1}{6} v_n^2 + \frac{1}{6} (7v_n - v_{n-1})^2,$$

$$\mathcal{R}_3[v_n] := \frac{1}{6} (\delta_1^2 v_n + \frac{1}{4} v_{n-1})^2;$$

- for $k = 4$, the constant $\sigma_{L4} := \frac{4919}{3072} \approx 1.601$,

$$\begin{aligned} \mathcal{G}_4[v_n] &:= \frac{3433}{6144}v_n^2 - \frac{15}{64}v_{n-1}^2 + \frac{1}{8}v_{n-2}^2 + \frac{47}{192}(\delta_1 v_n)^2 - \frac{3}{16}(\delta_1 v_{n-1})^2 \\ &+ \frac{3}{16}(\delta_1^2 v_n)^2 = \frac{13627}{43008}v_n^2 + \frac{7}{24}(\frac{65}{56}v_n - v_{n-1})^2 + \frac{1}{8}(\frac{3}{2}\delta_1 v_n + v_{n-2})^2, \\ \mathcal{R}_4[v_n] &:= \frac{1}{8}(\delta_1^3 v_n + \frac{3}{2}\delta_1 v_{n-1})^2 + \frac{1}{6}(\delta_1^2 v_n + \frac{35}{32}v_{n-1})^2; \end{aligned}$$

- for $k = 5$, the constant $\sigma_{L5} := \frac{646631}{1920000} \approx 0.3367$,

$$\begin{aligned} \mathcal{G}_5[v_n] &:= \frac{4227769}{3840000}v_n^2 - \frac{551}{1600}v_{n-1}^2 + \frac{17}{40}v_{n-2}^2 - \frac{1}{10}v_{n-3}^2 + \frac{1607}{4800}(\delta_1 v_n)^2 \\ &- \frac{39}{80}(\delta_1 v_{n-1})^2 + \frac{2}{5}(\delta_1 v_{n-2})^2 + \frac{7}{80}(\delta_1^2 v_n)^2 - \frac{2}{5}(\delta_1^2 v_{n-1})^2 + \frac{1}{5}(\delta_1^3 v_n)^2 \\ &= \frac{1198850903}{1678080000}v_n^2 + \frac{437}{900}(\frac{4931}{6992}v_n - v_{n-1})^2 \\ &+ \frac{9}{40}(\frac{23}{18}\delta_1 v_n + v_{n-2})^2 + \frac{1}{10}(2\delta_1 v_n + 2v_{n-2} - v_{n-3})^2, \\ \mathcal{R}_5[v_n] &:= \frac{(\delta_1^4 v_n + 2\delta_1^2 v_{n-1})^2}{10} + \frac{1}{8}(\delta_1^3 v_n + \frac{23}{10}\delta_1 v_{n-1})^2 + \frac{1}{6}(\delta_1^2 v_n + \frac{1787}{800}v_{n-1})^2. \end{aligned}$$

Thus the quadratic form $b_j^{(k)}$ associated with the BDF- k kernels can be re-strained by

$$2 \sum_{\ell=k}^n v_\ell \sum_{j=k}^{\ell} b_{\ell-j}^{(k)} v_j \geq \sigma_{Lk} \sum_{\ell=k}^n v_\ell^2 \quad \text{for } n \geq k.$$

We now prove the energy stability of BDF- k scheme (1.7). Let $E[\phi^n]$ be the discrete version of energy (Lyapunov) functional,

$$E[\phi^n] := \frac{\gamma}{2} \|\Delta_h \phi^n\|^2 + \frac{1}{2} \|\nabla_h \phi^n\|^2 + \frac{1}{4} \|(\phi^n)^2 - 1\|^2.$$

Define the following modified discrete energy $\mathcal{E}_k[\phi^n]$ and

$$\mathcal{E}_k[\phi^n] := E[\phi^n] + \frac{1}{\tau} \langle \mathcal{G}_k[\nabla_\tau \phi^n], 1 \rangle.$$

Due to the employment of BDF- k formula D_k , the above modified energy formula $\mathcal{E}_k[\phi^n]$ inserts a perturbed term which the term is $O(\tau)$ in the primal energy $E[\phi^n]$. Always, we assume that the modified discrete energy $\mathcal{E}_k[\phi^0]$, $\mathcal{E}_k[\phi^1]$, ..., $\mathcal{E}_k[\phi^{k-1}]$ satisfy the energy dissipation law. Next we will prove the following theorem.

Theorem 2. *If the time-step size τ fulfills*

$$\tau \leq \min \{b_0^{(k)}, \sigma_{Lk}\} \quad \text{for } n \geq k, \tag{2.1}$$

where $\sigma_{L3} \approx 1.979 > b_0^{(3)}$, $\sigma_{L4} \approx 1.601 < b_0^{(4)}$ and $\sigma_{L5} \approx 0.3367 < b_0^{(5)}$. Then the BDF- k implicit scheme (1.7) preserves the following energy dissipation law

$$\mathcal{E}_k[\phi^n] \leq \mathcal{E}_k[\phi^{n-1}] \quad \text{for } n \geq k.$$

Proof. Taking the inner product of (1.7) by $\nabla_\tau \phi^n$, for $n \geq k$, one has

$$\begin{aligned} & \langle D_k \phi^n, \nabla_\tau \phi^n \rangle + \gamma \langle \Delta_h \phi^n, \nabla_\tau \Delta_h \phi^n \rangle + \langle \nabla_h \phi^n, \nabla_\tau \nabla_h \phi^n \rangle \\ & + \langle (\phi^n)^3 - \phi^n, \nabla_\tau \phi^n \rangle = 0, \end{aligned} \quad (2.2)$$

which the discrete Green's formula has been used with periodic boundary conditions. Applying Lemma 2, one can obtain that

$$\langle D_k \phi^n, \nabla_\tau \phi^n \rangle \geq \frac{1}{\tau} \langle \mathcal{G}_k[\nabla_\tau \phi^n], 1 \rangle - \frac{1}{\tau} \langle \mathcal{G}_k[\nabla_\tau \phi^{n-1}], 1 \rangle + \frac{\sigma_{Lk}}{2\tau} \|\nabla_\tau \phi^n\|^2.$$

With the aid of the discrete Green's formula and $2a(a-b) = a^2 - b^2 + (a-b)^2$, one has

$$\begin{aligned} \gamma \langle \Delta_h \phi^n, \nabla_\tau \Delta_h \phi^n \rangle &= \frac{\gamma}{2} \|\Delta_h \phi^n\|^2 - \frac{\gamma}{2} \|\Delta_h \phi^{n-1}\|^2 + \frac{\gamma}{2} \|\nabla_\tau \Delta_h \phi^n\|^2, \\ \langle \nabla_h \phi^n, \nabla_\tau \nabla_h \phi^n \rangle &= \frac{1}{2} \|\nabla_h \phi^n\|^2 - \frac{1}{2} \|\nabla_h \phi^{n-1}\|^2 + \frac{1}{2} \|\nabla_\tau \nabla_h \phi^n\|^2. \end{aligned}$$

Noting the following relationship

$$\begin{aligned} 4(a^3 - a)(a - b) &= (a^2 - 1)^2 - (b^2 - 1)^2 - 2(1 - a^2)(a - b)^2 + (a^2 - b^2)^2 \\ &\geq (a^2 - 1)^2 - (b^2 - 1)^2 - 2(a - b)^2, \end{aligned}$$

then one can obtain

$$\langle (\phi^n)^3 - \phi^n, \nabla_\tau \phi^n \rangle \geq \frac{1}{4} \|(\phi^n)^2 - 1\|^2 - \frac{1}{4} \|(\phi^{n-1})^2 - 1\|^2 - \frac{1}{2} \|\nabla_\tau \phi^n\|^2.$$

Inserting the above results into (2.2) yields

$$\frac{1}{2} (\sigma_{Lk}/\tau - 1) \|\nabla_\tau \phi^n\|^2 + \mathcal{E}_k[\phi^n] \leq \mathcal{E}_k[\phi^{n-1}] \quad \text{for } n \geq k.$$

The time step restriction (2.1) implies the claimed discrete energy stable immediately. \square

Theorem 3. Assume the time-step size τ satisfies the condition (2.1), the numerical solution of the BDF-k scheme (1.7) is bounded (stable) in the L^∞ norm

$$\|\phi^n\|_\infty \leq c_0 := c_\Omega \sqrt{4\gamma^{-1}c_2 + (2 + \gamma)|\Omega_h|} \quad \text{for } n \geq k.$$

Similarly, the continuous energy dissipation law gives

$$\|\Phi(t_n)\|_\infty \leq \|\Phi(t_n)\|_{L^\infty} \leq c_1.$$

Note that, the fixed constant c_0 may dependent on the domain Ω , but c_0 is independent of the spatial length, the time steps τ and the current time t_n .

Proof. The result follows from the proof of [26, Lemma 3.3] in the same way. \square

3 L^2 norm convergence analysis

3.1 Some properties of the DOC kernels

The discrete convolution form (1.4) plays an important role in our convergence analysis, we give some properties of the DOC kernels and discrete convolution inequalities firstly, cf. [21, Lemma2.1] and [22, Lemma 2.5].

Lemma 3. *The discrete kernels $b_j^{(k)}$ in (1.2) are positive (semi-)definite if and only if the associated DOC-k kernels $\theta_j^{(k)}$ in (1.3) are positive (semi-)definite.*

Lemma 4. *For $3 \leq k \leq 5$, the associated DOC-k kernels $\theta_j^{(k)}$ defined in (1.3) are positive definite and satisfy the following decaying estimates*

$$|\theta_j^{(k)}| \leq \frac{\rho_k}{4} \left(\frac{k}{7}\right)^j \quad \text{for } j \geq 0,$$

where the constants $\rho_3 = 10/3$, $\rho_4 = 6$ and $\rho_5 = 96/5$.

3.2 L^2 norm error estimate

Now we are to establish the L^2 norm error estimate of the BDF-k scheme (1.7). Let the local consistency error at the time $t = t_j$,

$$\xi_{\Phi}^j := D_k \Phi(t_j) - \partial_t \Phi(t_j).$$

Consider a convolutional consistency error Ξ_{Φ}^k defined by

$$\Xi_{\Phi}^{\ell} := \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \xi_{\Phi}^j = \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} [D_k \Phi(t_j) - \partial_t \Phi(t_j)] \quad \text{for } \ell \geq k. \quad (3.1)$$

Then, we arrive at the following estimate on the convolutional consistency by Lemma 4.

Lemma 5. *For any $k \geq 3$, the convolutional consistency error Ξ_{Φ}^k in (3.1) satisfies $\|\xi^j\| \leq C_{\phi} \tau^k$, such that*

$$\sum_{\ell=k}^n \tau \|\Xi_{\Phi}^{\ell}\| \leq \frac{\rho_k t_{n-k+1}}{7-k} C_{\phi} \tau^k \quad \text{for } n \geq k.$$

Proof. By using the Taylor's expansion formula, one has

$$\begin{aligned} \xi^j &= \frac{1}{k! \tau} \sum_{l=1}^{k-1} (b_l - b_{l-1}) \int_{t_{j-l}}^{t_j} (t - t_{j-l})^k \Phi^{(k+1)}(t) dt \\ &\quad - \frac{1}{k! \tau} b_{k-1} \int_{t_{j-k}}^{t_j} (t - t_{j-l})^k \Phi^{(k+1)}(t) dt, \end{aligned}$$

so we have

$$\begin{aligned} \|\xi^j\| &\leq \frac{1}{k!} \tau^k \sum_{l=1}^{k-1} |b_l - b_{l-1}| \int_{t_{j-l}}^{t_j} \|\Phi^{(k+1)}(t)\| dt + \frac{1}{k!} |b_{k-1}| \tau^k \int_{t_{j-k}}^{t_j} \|\Phi^{(k+1)}(t)\| dt \\ &\leq C_\phi \tau^k \max_{t_k \leq t \leq T} |\partial_t^{(k+1)} \Phi(t)| \leq C_\phi \tau^k, \end{aligned}$$

and Lemma 4 yields the following estimate

$$\sum_{\ell=k}^n \tau \|\Xi_\Phi^\ell\| \leq C_\phi \tau^{k+1} \sum_{\ell=k}^n \sum_{j=k}^{\ell} |\theta_{\ell-j}^{(k)}| \leq \frac{\rho_k t_{n-k+1}}{7-k} C_\phi \tau^k \quad \text{for } n \geq k,$$

where C_ϕ is independent of the time step τ and time t_n , then the proof is completed. \square

Lemma 6. [22, Lemma 2.6] *There exist some positive constants $c_{1,k} > 1$ such that the starting values $\phi_1^{(k,j)}$ satisfy*

$$|\phi_1^{(k,j)}| \leq \frac{c_{1,k} \rho_k}{8} \left(\frac{k}{7}\right)^{j-k} \sum_{\ell=1}^{k-1} |\nabla_\tau \phi^\ell| \quad \text{for } 3 \leq k \leq 5 \text{ and } j \geq k,$$

such that

$$\sum_{j=k}^n |\phi_1^{(k,j)}| \leq \frac{7c_{1,k} \rho_k}{8(7-k)} \sum_{\ell=1}^{k-1} |\nabla_\tau \phi^\ell| \quad \text{for } 3 \leq k \leq 5 \text{ and } n \geq k,$$

where the constants ρ_k are defined in Lemma 4.

Theorem 4. *Suppose $\Phi \in C_{\mathbf{x},t}^{(4,6)}(\Omega \times (0, T])$ is a solution of the EFK problem (1.1) and the time-step condition (2.1) holds. Assume further that if the time step τ is small enough such that $\tau \leq \frac{7-k}{7\rho_k c_3}$, the solution ϕ^n of the BDF-k scheme (1.7) is convergent in the L^2 norm,*

$$\|\Phi^n - \phi^n\| \leq \frac{7\rho_k}{7-k} \exp\left(\frac{7\rho_k c_3}{7-k} t_{n-k+1}\right) \left[c_{1,k} \sum_{\ell=0}^{k-1} \|e^\ell\| + C_\phi t_{n-k+1} (\tau^k + h^2) \right]$$

for $k \leq n \leq N$.

Here, $c_3 := 1 + c_0^2 + c_0 c_1 + c_1^2$ is dependent on the domain Ω and the initial values Φ^0 and ϕ^0 , but independent of the time t_n , the time-step size τ and the spatial length h .

Proof. Let $e_h^n := \Phi_h^n - \phi_h^n$ for $\mathbf{x}_h \in \bar{\Omega}_h$. The local truncation error equation is obtained, such as

$$D_k e_h^j + \gamma \Delta_h^2 e_h^j - \Delta_h e_h^j + f(\Phi_h^j) - f(\phi_h^j) = \xi_h^j + \eta_h^j, \quad \mathbf{x}_h \in \Omega_h, \quad k \leq j \leq N, \quad (3.2)$$

where ξ_h^j is defined as the truncation error in time and η_h^j is denoted the error in space, respectively. Under the regularity setting of solution and Lemma 4, we conclude

$$\sum_{\ell=k}^n \tau \|\Upsilon^\ell\| \leq C_\phi \tau h^2 \sum_{\ell=k}^n \sum_{j=k}^{\ell} |\theta_{\ell-j}^{(k)}| \leq \frac{\rho_k t_{n-k+1}}{7-k} C_\phi h^2 \quad \text{for } k \leq n \leq N, \quad (3.3)$$

where $\Upsilon_h^\ell := \sum_{j=k}^{\ell} \theta_{k-j}^{(k)} \eta_h^j$ for $\ell \geq k$.

Multiplying both sides of (3.2) by the DOC kernels $\tau \theta_{\ell-j}^{(k)}$, and summing up the superscript from $j = k$ to ℓ we apply the identity (1.8) to obtain

$$\begin{aligned} \nabla_\tau e^\ell + \tau \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} (\gamma \Delta_h^2 - \Delta_h) e_h^j &= -e_I^{(k,\ell)} + \tau \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} [f(\phi_h^j) - f(\Phi_h^j)] \\ &+ \tau \Upsilon_h^\ell + \tau \Xi^\ell, \end{aligned} \quad (3.4)$$

where $e_I^{(k,n)}$ represents the starting error effects on the numerical solution at the time t_n ,

$$e_I^{(k,n)} := \sum_{\ell=1}^{k-1} \nabla_\tau e^\ell \sum_{j=k}^n \theta_{n-j}^{(k)} b_{j-\ell}^{(k)} \quad \text{for } n \geq k. \quad (3.5)$$

Making the inner product of the above equality (3.4) with $2e^\ell$, and summing up the superscript from k to n , one can apply the discrete Green's formula to derive that

$$\begin{aligned} \|e^n\|^2 - \|e^{k-1}\|^2 + 2 \sum_{\ell=k}^n \langle e_I^{(k,\ell)}, e^\ell \rangle + J^n \\ \leq 2\tau \sum_{\ell,j}^{n,\ell} \theta_{\ell-j}^{(k)} \langle f(\phi_h^j) - f(\Phi_h^j), e^\ell \rangle + 2\tau \sum_{\ell=k}^n \langle \Upsilon_h^\ell + \Xi^\ell, e^\ell \rangle \end{aligned} \quad (3.6)$$

for $k \leq n \leq N$, where J^n is defined by

$$J^n := 2\gamma\tau \sum_{\ell,j}^{n,\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, \Delta_h e^\ell \rangle + 2\tau \sum_{\ell,j}^{n,\ell} \theta_{\ell-j}^{(k)} \langle \nabla_h e^j, \nabla_h e^\ell \rangle.$$

The positive definiteness of DOC kernels in Lemma 3 shows that the term $J^n > 0$. By virtue of the maximum norm estimates in Theorem 3, we have

$$|f(\phi_h^j) - f(\Phi_h^j)| = |(\phi_h^j)^2 + \phi_h^j \Phi_h^j + (\Phi_h^j)^2 - 1| |e_h^j| \leq c_3 |e_h^j|.$$

Then, it follows from (3.6) that

$$\begin{aligned} \|e^n\|^2 \leq \|e^{k-1}\|^2 + 2 \sum_{\ell=k}^n \|e_I^{(k,\ell)}\| \|e^\ell\| + 2c_3\tau \sum_{\ell=k}^n \theta_{\ell-j}^{(k)} \|e^j\| \|e^\ell\| \\ + 2\tau \sum_{\ell=k}^n \|e^\ell\| \|\Upsilon^\ell + \Xi^\ell\|. \end{aligned} \quad (3.7)$$

Choose some integer n_0 ($k-1 \leq n_0 \leq n$) such that $\|e^{n_0}\| = \max_{k-1 \leq \ell \leq n} \|e^j\|$. Let $n = n_0$ in the above inequality (3.7), one gets

$$\begin{aligned} \|e^{n_0}\| &\leq \|e^{k-1}\| + 2 \sum_{\ell=k}^{n_0} \|e_1^{(k,\ell)}\| + 2c_3\tau \sum_{\ell=k}^{n_0} \sum_{j=k}^{\ell} \|\theta_{\ell-j}^{(k)} e^\ell\| + 2\tau \sum_{\ell=k}^{n_0} \|\Upsilon^\ell + \Xi^\ell\| \\ &\leq \|e^{k-1}\| + 2 \sum_{\ell=k}^n \|e_1^{(k,\ell)}\| + 2c_3\tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} |\theta_{\ell-j}^{(k)}| \|e^\ell\| + 2\tau \sum_{\ell=k}^n \|\Upsilon^\ell + \Xi^\ell\|. \end{aligned} \tag{3.8}$$

Applying Lemma 6 to the starting term $e_1^{(k,\ell)}$ in (3.5), one has

$$2 \sum_{\ell=k}^n \|e_1^{(k,\ell)}\| \leq \frac{7c_{1,k}\rho_k}{4(7-k)} \sum_{\ell=1}^{k-1} \|\nabla_\tau e^\ell\| \quad \text{for } k \leq n \leq N.$$

For the right term in (3.8), one can derive the following estimates in a similar fashion

$$2c_3\tau \sum_{j=k}^n \sum_{\ell=k}^j |\theta_{\ell-j}^{(k)}| \|e^\ell\| \leq \frac{\rho_k}{2} c_3\tau \sum_{j=k}^n \sum_{\ell=k}^j \left(\frac{k}{7}\right)^{j-\ell} \|e^\ell\| \leq \frac{7\rho_k}{2(7-k)} c_3\tau \sum_{\ell=k}^n \|e^\ell\|.$$

Thus, we can use Lemma 4 to get the following estimate

$$\|e^n\| \leq \|e^{n_0}\| \leq \frac{7c_{1,k}\rho_k}{2(7-k)} \sum_{\ell=0}^{k-1} \|e^\ell\| + \frac{7\rho_k c_3}{2(7-k)} \tau \sum_{\ell=k}^n \|e^\ell\| + 2\tau \sum_{\ell=k}^n \|\Upsilon^m + \Xi^m\|.$$

Under the time-step constraint $\tau \leq \frac{7-k}{7\rho_k c_3}$, one has

$$\|e^n\| \leq \frac{7c_{1,k}\rho_k}{7-k} \sum_{\ell=0}^{k-1} \|e^\ell\| + \frac{7\rho_k c_3}{7-k} \tau \sum_{\ell=k}^{n-1} \|e^\ell\| + 4\tau \sum_{\ell=k}^n \|\Upsilon^m + \Xi^m\|.$$

Obviously, applying the discrete Grönwall inequality, one can obtain

$$\|e^n\| \leq \exp\left(\frac{7\rho_k c_3}{7-k} t_{n-k+1}\right) \left[\frac{7c_{1,k}\rho_k}{7-k} \sum_{\ell=0}^{k-1} \|e^\ell\| + 4\tau \sum_{\ell=k}^n \|\Upsilon^m + \Xi^m\| \right]$$

for $k \leq n \leq N$. The proof is completed from Lemma 5 and the error estimate (3.3). \square

4 Numerical example

In this section, we will verify our conclusions with numerical examples. We employ the sixth-order implicit Runge-Kutta method to initiate the numerical schemes. In all our computations, a fixed-point iteration scheme will be employed to solve the nonlinear scheme at each time level with a tolerance 10^{-10} .

4.1 Accuracy test

Example 1. We set $\gamma = 0.02$ and consider the following exterior-forced EFK model

$$\partial_t \Phi + \gamma \Delta^2 \Phi - \Delta \Phi + f(\Phi) = g(\mathbf{x}, t)$$

for $\mathbf{x} \in (0, \pi)^2$ such that it has exact solution $\Phi = \cos(t) \sin(2x) \sin(2y)$.

The computational domain $(0, \pi)^2$ is discretized by using 256^2 spatial meshes and solve the problem until $T = 1$. The numerical results are listed in Tables 2–4, where the discrete L^2 norm error $e(N) := \|\Phi(T) - \phi^N\|$ is recorded in each run and the experimental order of convergence is computed by

$$\text{Order} \approx \frac{\log(e(N)/e(2N))}{\log(\tau(N)/\tau(2N))}.$$

Table 2. Accuracy of BDF3 scheme.

N	τ	$e(N)$	Order
15	6.67e-02	7.25e-04	–
30	3.33e-02	8.68e-05	3.06
60	1.67e-02	1.06e-05	3.03
120	8.33e-03	1.31e-06	3.02
240	4.17e-03	1.63e-07	3.01

Table 3. Accuracy of BDF4 scheme.

N	τ	$e(N)$	Order
15	6.67e-02	3.95e-05	–
30	3.33e-02	2.60e-06	3.92
60	1.67e-02	1.67e-07	3.96
120	8.33e-03	1.05e-08	3.98
240	4.17e-03	6.63e-10	3.99

Table 4. Accuracy of BDF5 scheme.

N	τ	$e(N)$	Order
15	6.67e-02	2.27e-06	–
30	3.33e-02	6.66e-08	5.09
60	1.67e-02	2.00e-09	5.06
120	8.33e-03	6.27e-11	5.00
240	4.17e-03	1.88e-12	5.06

From these data it can be observed that the BDF- k scheme admits k -th order accuracy.

4.2 Numerical application

Example 2. We consider the EFK model (1.1) with the following initial data

$$\Phi(\mathbf{x}, 0) = 0.1 (\sin(3x) \sin(2y) + \sin(5x) \sin(5y)).$$

We take the model parameter $\gamma = 10^{-4}$ and use 128^2 uniform mesh to discretize the spatial domain $(0, 2\pi)^2$.

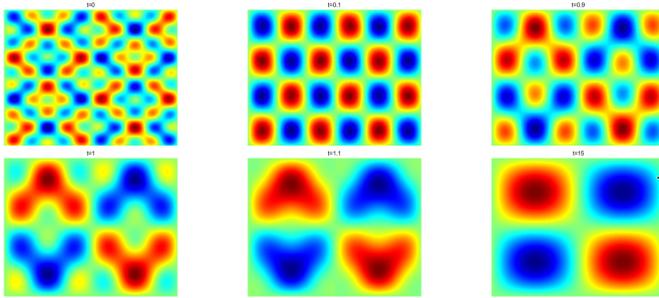


Figure 1. Solution snapshots of the BDF3 scheme for the EFK equation at $t = 0, 0.1, 0.9, 1, 1.1, 15$, respectively (the BDF-4 and BDF-5 schemes generate similar profiles).

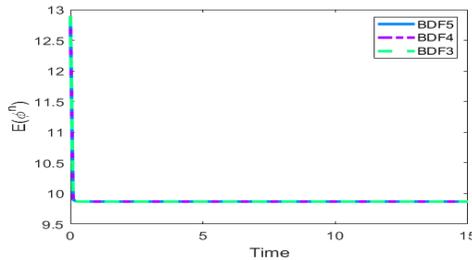


Figure 2. Evolutions of original energy of the BDF-K scheme for the EFK equation.

We here begin with the examination using a constant time step $\tau = 10^{-3}$ until time $T = 15$ (i.e., $N = 15000$). The evolution of phase variable is presented in Figure 1. One can find that the initial solution evolve on a fast time scale while later ones evolve on a very slow time scale. The evolution of the original energy $E[\phi^n]$ over time is shown in Figure 2, and it can be seen that during the coarsening process, the free energy decays monotonically.

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