A new discrete energy technique for multi-step backward difference formulas

Hong-lin Liao* Tao Tang† Tao Zhou‡

February 10, 2021

Abstract

The backward differentiation formula (BDF) is a useful family of implicit methods for the numerical integration of stiff differential equations. It is well noticed that the stability and convergence of the $A$-stable BDF1 and BDF2 schemes for parabolic equations can be directly established by using the standard discrete energy analysis. However, such classical analysis technique seems not directly applicable to the BDF-$k$ schemes for $3 \leq k \leq 5$. To overcome the difficulty, a powerful analysis tool based on the Nevanlinna-Odeh multiplier technique [Numer. Funct. Anal. Optim., 3:377-423, 1981] was developed by Lubich et al. [IMA J. Numer. Anal., 33:1365-1385, 2013]. In this work, by using the so-called discrete orthogonal convolution kernels technique, we will recover the classical energy analysis so that the stability and convergence of the BDF-$k$ schemes for $3 \leq k \leq 5$ can be established. One of the theoretical advantages of our analysis technique is that less spacial regularity requirement is needed on the initial data.

Keywords: linear diffusion equations, backward differentiation formulas, discrete orthogonal convolution kernels, positive definiteness, stability and convergence.

AMS subject classifications: 65M06, 65M12

1 Introduction

The backward differentiation formula (BDF) is a family of implicit methods for the numerical integration of stiff differential equations. They are linear multistep methods that approximate the derivative of the unknown function using information from already computed time points,
thereby increasing the accuracy of the approximation. These methods are especially used for the solution of stiff differential equations whose numerical stability is indicated by the region of absolute stability. More precisely, if the region of stability contains the left half of the complex plane, then the method is said to be $A$-stable. It is known that backward differentiation methods with an order greater than 2 cannot be $A$-stable, i.e., only the first-order and second-order backward differentiation formulas (i.e., BDF1 and BDF2) are $A$-stable. For parabolic equations, it is also well-known that the energy stability and convergence of $A$-stable BDF1 and BDF2 methods can be established by using the standard discrete energy analysis, see, e.g., [14].

However, this standard analysis technique is not directly applicable to higher order BDF schemes. This results in several remedies to recover the $L^2$-norm stability and convergence for the non-$A$-stable $k$-step backward difference formulas with $3 \leq k \leq 5$. It is particularly noted that due to the seminal work of Lubich et al. [12], the Nevanlinna-Odeh multiplier technique [13] has been successfully used for this purpose, see e.g. [1]–[4] and references therein. The key idea of such a multiplier technique relies on the equivalence between $A$-stability and $G$-stability of Dahlquist [5]. Another useful tool for the numerical analysis of BDF-$k$ schemes is the telescope formulas by Liu [11], which is also based on the Dahlquist’s $G$-stability theory [5].

We have a natural question: is there a straightforward discrete energy analysis for the BDF-$k$ schemes with $3 \leq k \leq 5$? The aim of this work is to provide a definite answer by introducing a novel yet straightforward discrete energy method based on the so-called discrete orthogonal convolution (DOC) kernel technique [10]. To this end, we consider the linear reaction-diffusion problem in a bounded convex domain $\Omega$,

$$\partial_t u - \varepsilon \Delta u = \beta(x,t) u + f(t,x), \quad x \in \Omega, \quad 0 < t < T,$$

subject to the Dirichlet boundary condition $u = 0$ on a smooth boundary $\partial \Omega$. The initial data is set to be $u(0,x) = u_0(x)$. We assume that the diffusive coefficient $\varepsilon > 0$ is a constant and the reaction coefficient $\beta(x,t)$ is smooth and bounded by $\beta^* > 0$.

Let $t_k = k \tau$ be an uniform discrete time-step with $\tau := T/N$. For any discrete time sequence $\{v^n\}_{n=0}^N$, we denote

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

For a fixed index $3 \leq k \leq 5$, we shall view the BDF-$k$ formula $D_k v^n$ as a discrete convolution summation as follows

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

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

$$\sum_{\ell=1}^k \frac{1}{\ell} (1 - \zeta)^{\ell-1} = \sum_{\ell=0}^{k-1} b^{(k)}_\ell \zeta^\ell, \quad 3 \leq k \leq 5.\quad(1.3)$$

To make our idea clear, the initial data $u^1, u^2, \cdots, u^{k-1}$ for the multi-step BDF-$k$ schemes ($3 \leq k \leq 5$) are assumed to be available. Without loss of generality, we consider the time-discrete solution, $u^k(x) \approx u(t_k, x)$ for $x \in \Omega$, defined by the following implicit multi-step BDF scheme

$$D_k w^j = \varepsilon \Delta w^j + \beta^j w^j + f^j, \quad k \leq j \leq N,$$

subject to the boundary condition $w^j = 0$ on the smooth boundary $\partial \Omega$. The initial data is set to be $w^0 = u^k$. We assume that the diffusive coefficient $\varepsilon > 0$ is a constant and the reaction coefficient $\beta^j(x,t)$ is smooth and bounded by $\beta^{*j} > 0$. For a fixed index $3 \leq k \leq 5$, we shall view the BDF-$k$ formula $D_k w^j$ as a discrete convolution summation as follows

$$D_k w^j := \frac{1}{\tau} \sum_{k=1}^j b^{(k)}_{j-k} \nabla_{\tau} w^k, \quad j \geq k,$$

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

$$\sum_{\ell=1}^k \frac{1}{\ell} (1 - \zeta)^{\ell-1} = \sum_{\ell=0}^{k-1} b^{(k)}_\ell \zeta^\ell, \quad 3 \leq k \leq 5.\quad(1.3)$$

To make our idea clear, the initial data $w^1, w^2, \cdots, w^{k-1}$ for the multi-step BDF-$k$ schemes ($3 \leq k \leq 5$) are assumed to be available. Without loss of generality, we consider the time-discrete solution, $w^k(x) \approx u(t_k, x)$ for $x \in \Omega$, defined by the following implicit multi-step BDF scheme

$$D_k w^j = \varepsilon \Delta w^j + \beta^j w^j + f^j, \quad k \leq j \leq N,$$
Then by acting the associated DOC kernels \( \theta \)

\[
\delta \theta \text{ discrete orthogonal convolution identity holds } [9,10]: \\
\sum_{j} \quad 
\]

Here and hereafter, we set \( \text{form. For the discrete BDF-} k \text{ form of (1.5) using the DOC kernels technique. Below we will derive the equivalent convolution steps) was investigated. More precisely, our analysis will be based on an equivalent convolution form of (1.5) using the DOC kernels technique. Below we will derive the equivalent convolution form. For the discrete BDF-} k \text{ kernels } b_{j}^{(k)} \text{ generated by (1.3), the corresponding DOC-} k \text{ kernels } \theta_{j}^{(k)} \text{ are defined recursively as:}

\[
\theta_{0}^{(k)} := \frac{1}{b_{0}^{(k)}} \quad \text{and} \quad \theta_{n-j}^{(k)} := -\frac{1}{b_{0}^{(k)}} \sum_{\ell=j+1}^{n} \theta_{n-\ell}^{(k)} b_{\ell-j}^{(k)} \quad \text{for } j = n - 1, n - 2, \cdots, k. 
\]

Here and hereafter, we set \( \sum_{k=i}^{j} \cdot = 0 \) whenever \( i > j \). It is easy to check that the following \textit{discrete orthogonal convolution identity} holds [9,10]:

\[
\sum_{\ell=j}^{n} \theta_{n-\ell}^{(k)} b_{\ell-k}^{(k)} \equiv \delta_{nj} \quad \text{for } \forall \ k \leq j \leq n, 
\]

where \( \delta_{nk} \) is the Kronecker delta. Thus, by exchanging the summation index, one gets

\[
\sum_{j=k}^{n} \theta_{n-j}^{(k)} \sum_{\ell=k}^{j} b_{j-\ell}^{(k)} \nabla_{\tau} u_{\ell} = \sum_{\ell=k}^{n} \nabla_{\tau} u_{\ell} \sum_{j=k}^{n} \theta_{n-j}^{(k)} b_{j-\ell}^{(k)} = \nabla_{\tau} u_{n}, \quad k \leq n \leq \mathcal{N}.
\]

Then by acting the associated DOC kernels \( \theta_{n-j}^{(k)} \) on the BDF-} k formula \( D_{k} \), we obtain

\[
\sum_{j=k}^{n} \theta_{n-j}^{(k)} D_{k} u_{j} = \frac{1}{\tau} \sum_{j=k}^{n} \theta_{n-j}^{(k)} \sum_{\ell=1}^{k-1} b_{j-\ell}^{(k)} \nabla_{\tau} u_{\ell} + \frac{1}{\tau} \sum_{j=k}^{n} \theta_{n-j}^{(k)} \sum_{\ell=k}^{j} b_{j-\ell}^{(k)} \nabla_{\tau} u_{\ell} \\
\triangleq \frac{1}{\tau} u_{1}^{(k,n)} + \partial_{\tau} u_{n} \quad \text{for } k \leq n \leq \mathcal{N}, 
\]

\( \text{Table 1: The BDF-} k \text{ kernels } b_{j}^{(k)} \text{ generated by (1.3)} \)

| BDF-} k | \( b_{0}^{(k)} \) | \( b_{1}^{(k)} \) | \( b_{2}^{(k)} \) | \( b_{3}^{(k)} \) | \( b_{4}^{(k)} \) |
|--------|--------|--------|--------|--------|--------|
| \( k = 2 \) | 3 \( \frac{7}{2} \) | -1 \( \frac{7}{2} \) | 137 \( \frac{137}{60} \) | -4 \( \frac{21}{20} \) | 1 \( \frac{1}{5} \) |
| \( k = 3 \) | 11 \( \frac{137}{12} \) | -7 \( -\frac{7}{6} \) | 25 \( -\frac{25}{12} \) | 12 \( \frac{25}{12} \) | -3 \( \frac{1}{4} \) |
| \( k = 4 \) | 3 \( \frac{25}{12} \) | -4 \( -\frac{24}{12} \) | 13 \( \frac{13}{12} \) | 12 \( \frac{13}{12} \) | -3 \( \frac{1}{4} \) |
| \( k = 5 \) | 25 \( \frac{137}{60} \) | -63 \( -\frac{63}{60} \) | 25 \( \frac{25}{60} \) | 25 \( -\frac{25}{60} \) | -4 \( -\frac{4}{5} \) |

where \( f^{j}(x) = f(t_{j}, x) \). The weak form of (1.4) reads

\[
\langle D_{k} u^{j}, w \rangle + \varepsilon \langle \nabla u^{j}, \nabla w \rangle = \langle \beta^{j} u^{j}, w \rangle + \langle f^{j}, w \rangle \quad \text{for } \forall \ w \in H_{0}^{1}(\Omega) \text{ and } k \leq j \leq \mathcal{N}. 
\]

Here \( \langle \cdot, \cdot \rangle \) and \( || \cdot || \) are the \( L^{2} \) inner product and the \( L^{2} \)-norm, respectively.

Our new energy analysis for BDF-} k schemes with \( 3 \leq k \leq 5 \) relies on the discrete orthogonal convolution (DOC) kernels technique developed in [10], where the BDF2 scheme (with variable steps) was investigated. More precisely, our analysis will be based on an equivalent convolution form of (1.5) using the DOC kernels technique. Below we will derive the equivalent convolution form. For the discrete BDF-} k kernels \( b_{j}^{(k)} \) generated by (1.3), the corresponding DOC-} k kernels \( \theta_{j}^{(k)} \) are defined recursively as:
where \( u_1^{(k,n)} \) represents the starting effects on the numerical solution at \( t_n \), i.e.,

\[
u_1^{(k,n)} := \sum_{\ell=1}^{k-1} \nabla \tau u_\ell \sum_{j=k}^{n} \theta^{(k)}_{n-j} \theta^{(k)}_{j-\ell} \quad \text{for } n \geq k. \tag{1.9}\]

Now, by acting the associated DOC-k kernels \( \theta^{(k)}_{n-j} \) on the time-discrete problem \( (1.5) \), we use \( (1.8) \) and \( (1.9) \) to obtain

\[
\langle \partial_\tau u^j, w \rangle + \varepsilon \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle \nabla u^\ell, \nabla w \rangle = - \frac{1}{\tau} \langle u_1^{(k,j)}, w \rangle + \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle \beta^\ell u^\ell, w \rangle + \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle f^\ell, w \rangle
\]

for \( \forall \ w \in H_0^1(\Omega) \) and \( k \leq j \leq N. \tag{1.10}\]

This convolution formulation will be the starting point of our energy technique, and will lead to much more concise \( L^2 \)-norm estimates than those in previous works.

Note that, the DOC-k kernels define a \textit{reversible discrete transform} between the original form \( (1.5) \) and the convolution form \( (1.10) \). By following the proof of \cite{9} Lemma 2.1, it is easy to check

\[
\sum_{\ell=j}^{n} b^{(k)}_{n-\ell} \theta^{(k)}_{\ell-j} \equiv \delta_{mk} \quad \text{for } k \leq j \leq n. \tag{1.11}\]

Similar as the classical discrete \( L^2 \)-norm analysis, we can now take \( w = 2\tau u^j \) in \( (1.10) \) and sum up from \( j = k \) to \( n \) to obtain

\[
\| u^n \|^2 - \| u^{k-1} \|^2 \leq - 2 \sum_{j=k}^{n} \langle u_1^{(k,j)}, u^j \rangle - 2\varepsilon \tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle \nabla u^\ell, \nabla u^j \rangle
\]

\[
+ 2\tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle \beta^\ell u^\ell, u^j \rangle + 2\tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle f^\ell, u^j \rangle, \tag{1.12}\]

where the term \( \sum_{j=k}^{n} \| u^j - u^{j-1} \|^2 \) has been dropped in the left hand side. Consequently, we need to carefully handle the right hand side of \( (1.12) \), which consists the following issues:

- Positive definiteness of the DOC kernels \( \theta^{(k)}_j \) (see Section 2.1);
- Decay estimates of the DOC kernels \( \theta^{(k)}_j \) (see Section 2.2);
- Decay estimates of the initial term \( u_1^{(k,j)} \) (see Section 2.3).

By doing this, we can finally present concise stability and error estimates of \( (1.4) \) for the linear reaction-diffusion \( (1.1) \). More precisely, we show in Theorem \( 3.2 \) that, if the time-step size \( \tau \leq (7 - k)/(7\rho_k\beta^*) \), the time-discrete solution \( u^n \) is unconditionally stable in \( L^2 \)-norm:

\[
\| u^n \| \leq \frac{7\rho_k}{7 - k} \exp \left( \frac{7\rho_k}{7 - k} \beta^* t_{n-k} \right) \left( c_{1,k} \sum_{\ell=0}^{k-1} \| u^\ell \| + \sum_{\ell=k}^{n} \tau \| f^\ell \| \right) \quad \text{for } k \leq n \leq N,
\]
where the constants $\rho_k$ and $c_{1,k}$ are defined in Lemmas 2.5 and 2.6, respectively. This is followed by Theorem 3.3 which presents a concise $L^2$-norm error estimate for the BDF-$k$ schemes:

$$
\|u(t_n) - u^n\| \leq \frac{7\rho_k c_{1,k}}{7 - k} \exp\left(\frac{7\rho_k \beta^* t_n - k}{7 - k}\right) \left(\sum_{\ell=0}^{k-1} \|u(t_{\ell}) - u^\ell\| + C u t_{n-k} \tau^k\right).
$$

The paper is organized as follows. Section 2 contains several properties for the DOC-$k$ kernels which will be useful for the stability and convergence analysis. The main results outlined above will be proved in Section 3. Some concluding remarks will be given in the last section.

## 2 Preliminary results

In this section, we present several preliminary results which will be used for proving our main results in Section 3.

### 2.1 Positive definiteness of DOC-$k$ kernels

By using the mutual orthogonal identities (1.7) and (1.11), we have the following result on the positive definiteness, see [9, Lemma 2.1].

**Lemma 2.1** The discrete kernels $b^{(k)}_j$ in (1.3) are positive (semi-)definite if and only if the associated DOC kernels $\theta^{(k)}_j$ in (1.6) are positive (semi-)definite.

It remains to study the positive definiteness of discrete BDF-$k$ kernels. To this end, we introduce the Toeplitz form $T_m = (t_{ij})_{m \times m}$, where the entries $t_{ij} = t_{i-j}(i, j = 1, 2, \cdots, m)$ are constants along the diagonal of $T_m$. Let $t_k$ be the Fourier coefficients of the trigonometric polynomial $f$, i.e.,

$$
t_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ikx} \, dx, \quad k = 1 - m, 2 - m, \cdots, m - 1,
$$

where $i := \sqrt{-1}$ is the complex unit. Then

$$
f(x) = \sum_{k=1-m}^{m-1} t_k e^{ikx} \quad \text{is called the generating function of } T_m.
$$

(2.1)

The following Grenander-Szegö theorem [6, pp. 64–65] shows the relationship between the eigenvalues of $T_m$ and the generating function $f$.

**Lemma 2.2** Let $T_m = (t_{i-j})_{m \times m}$ be the Toeplitz matrix generated by the function $f$ defined in (2.1). Then the smallest eigenvalue $\lambda_{\min}(T_m)$ of $T_m$ and the largest one $\lambda_{\max}(T_m)$ can be bounded by

$$
f_{\min} \leq \lambda_{\min}(T_m) \leq \lambda_{\max}(T_m) \leq f_{\max},
$$

where $f_{\min}$ and $f_{\max}$ denote the minimum and maximum values of $f(x)$, respectively. Specially, the Toeplitz matrix $T_m$ is positive definite if $f_{\min} > 0$.
Now, for the BDF-k formula, we consider the following matrices of order $m := n - k + 1:

$$B_{k,l} := \begin{pmatrix}
\vdots & & & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
b_0^{(k)} & \cdots & b_0^{(k)} & b_0^{(k)} \\
b_1^{(k)} & \cdots & b_1^{(k)} & b_1^{(k)} \\
b_{k-1}^{(k)} & \cdots & b_{k-1}^{(k)} & b_{k-1}^{(k)} \\
b_k^{(k)} & \cdots & b_k^{(k)} & b_k^{(k)}
\end{pmatrix}_{m \times m}$$

and $B_k := B_{k,l} + B_{k,l}^T$, \hspace{1cm} (2.2)

where $3 \leq k \leq 5$ and the index $n \geq k$. According to definition (2.1), we define the generating function of $B_k$ as follows,

$$g^{(k)}(\varphi) = 2 \sum_{j=0}^{k-1} b_j^{(k)} \cos(j\varphi). \hspace{1cm} (2.3)$$

Consequently, Lemma 2.2 implies the following result.

**Lemma 2.3** Let $B_k$ be the real symmetric matrix generated by the function $g^{(k)}$ defined in (2.3). Then the smallest eigenvalue $\lambda_{\min}(B_k)$ and the largest one $\lambda_{\max}(B_k)$ can be bounded by

$$g_{\min}^{(k)} \leq \lambda_{\min}(B_k) \leq \lambda_{\max}(B_k) \leq g_{\max}^{(k)},$$

where $g_{\min}^{(k)}$ and $g_{\max}^{(k)}$ denote the minimum and maximum values of $g^{(k)}(\varphi)$, respectively. Specially, the real symmetric matrix $B_k$ is positive definite if $g_{\min}^{(k)} > 0$.

Now we apply Lemma 2.3 to establish the positive definiteness of the discrete BDF-k kernels $b_j^{(k)}$ for $3 \leq k \leq 5$, by investigating the associated generating functions $g^{(k)}(\varphi)$.

**Lemma 2.4** For the discrete BDF-k kernels $b_j^{(k)}$ ($3 \leq k \leq 5$) defined in (1.3) and any real sequence $\{w_k\}_{k=1}^n$ with $n$ entries, it holds that

$$2 \sum_{m=k}^n w_m \sum_{j=k}^m b_{m-j}^{(k)} w_j \geq \sigma_k \sum_{k=1}^n w_k^2 \text{ for } n \geq k,$$

where $\sigma_3 = 95/48 \approx 1.979$, $\sigma_4 = 1.628$ and $\sigma_5 = 0.4776$. Thus the discrete BDF-k kernels $b_j^{(k)}$ for $3 \leq k \leq 5$ are positive definite.

**Proof** Consider the real symmetric matrix $B_k$ in (2.2) of order $m := n - k + 1$. By setting $w := (w_k, w_{k+1}, \ldots, w_n)^T$ one obtains

$$2 \sum_{m=k}^n w_m \sum_{j=k}^m b_{m-j}^{(k)} w_j = w^T B_k w \geq \lambda_{\min}(B_k) w^T w \text{ for } n \geq k.$$

Thanks to Lemma 2.3, it remains to prove $g_{\min}^{(k)} \geq \sigma_k$. The associated generating functions (see Figure 1 for the function curves) are listed below:
\[ g^{(3)}(\varphi) = \frac{1}{3}(11 - 7 \cos \varphi + 2 \cos 2\varphi), \]

\[ g^{(4)}(\varphi) = \frac{1}{6}(25 - 23 \cos \varphi + 13 \cos 2\varphi - 3 \cos 3\varphi), \]

\[ g^{(5)}(\varphi) = \frac{1}{30}(137 - 163 \cos \varphi + 137 \cos 2\varphi - 63 \cos 3\varphi + 12 \cos 4\varphi). \]

Figure 1: Curves of generating functions \( g^{(k)}(\varphi) \) over \( \varphi \in [-\pi, \pi] \) for \( 3 \leq k \leq 5 \).

**I** The case \( k = 3 \). By the formula \( \cos 2\varphi = 2 \cos^2 \varphi - 1 \), we get

\[ g^{(3)}(\varphi) = \frac{1}{3}(9 - 7 \cos \varphi + 4 \cos^2 \varphi) = \frac{4}{3}(\cos \varphi - 7/8)^2 + \frac{95}{48}. \]

As desired, \( g^{(3)}_\text{min} = \sigma_3 = 95/48 \approx 1.97919 \).

**II** The case \( k = 4 \). By the formula \( \cos 3\varphi = 4 \cos^3 \varphi - 3 \cos \varphi \), we get

\[ g^{(4)}(\varphi) = \frac{1}{6}(12 - 14 \cos \varphi + 26 \cos^2 \varphi - 12 \cos^3 \varphi). \]

Consider a function \( Z_4(x) = 12 - 14x + 26x^2 - 12x^3 \). The first derivative \( Z'_4 = -14 + 52x - 36x^2 \) has a unique zero-point \( x^* = (13 - \sqrt{43})/18 \) for \( x \in [-1, 1] \). Then

\[ (Z_4)_{\text{min}} = \min\{Z_4(-1), Z_4(x^*), Z_4(1)\} = Z_4(x^*) = (2656 - 43\sqrt{43})/243. \]

Thus, we have

\[ g^{(4)}(\varphi) \geq \frac{1}{6}Z_4(x^*) = \frac{2656 - 43\sqrt{43}}{1458} \approx 1.62828. \]

**III** The case \( k = 5 \). By the formula \( \cos 4\varphi = 8 \cos^4 \varphi - 8 \cos^2 \varphi + 1 \), we get

\[ g^{(5)}(\varphi) = \frac{1}{30}(12 + 26 \cos \varphi + 178 \cos^2 \varphi - 252 \cos^3 \varphi + 96 \cos^4 \varphi). \]

Consider the following function \( Z_5(x) = 12 + 26x + 178x^2 - 252x^3 + 96x^4 \). The first derivative \( Z'_5 = 26 + 356x - 756x^2 + 384x^3 \) has a unique real zero-point \( x^* \) over the interval \([-1, 1]\),

\[ x^* = \frac{1}{96} \left( 63 - \sqrt[3]{49041 - 16\sqrt{3891895}} - \frac{1121}{\sqrt[3]{49041 - 16\sqrt{3891895}}} \right) \approx -0.064041. \]
Then
\[(Z_5)_{\text{min}} = \min\{Z_5(-1), Z_5(x^*), Z_5(1)\} = Z_5(x^*) \approx 14.3305.\]
Thus, we have
\[g^{(5)}(\varphi) \geq \frac{1}{30} Z_5(x^*) \approx 0.477683.\]
The proof is completed.

2.2 Decay estimates of DOC-\(k\) kernels

We now present the decay estimates of DOC-\(k\) kernels. Notice that although the BDF-\(k\) kernels \(b_j^{(k)}\) vanish for \(j \geq k\), the associated DOC-\(k\) kernels \(\theta_j^{(k)}\) are always nonzero for any \(j \geq 0\). The following lemma presents the decay property of the DOC-\(k\) kernels (we plot in Figure 2 the decay properties of those kernels).

![Figure 2: The DOC-\(k\) kernels and the bound \(\rho_k(x) = \frac{\rho_k}{4} \left(\frac{k}{7}\right)^x\) for 3 \(\leq\) \(k\) \(\leq\) 5.](image)

Lemma 2.5 The associated DOC-\(k\) kernels \(\theta_j^{(k)}\) defined in (1.6) satisfy
\[|\theta_j^{(k)}| \leq \frac{\rho_k}{4} \left(\frac{k}{7}\right)^j\]
for 3 \(\leq\) \(k\) \(\leq\) 5 and \(j \geq 0\),
where \(\rho_3 = 10/3\), \(\rho_4 = 6\) and \(\rho_5 = 96/5\).

Proof By the definition (1.6), we have \(\theta_0^{(k)} = 1/b_0^{(k)}\) and \(\sum_{j=0}^{n} \theta_j^{(k)} b_{n-j}^{(k)} = 0\) (\(k \leq j \leq n-1\)),
or,
\[\sum_{m=0}^{j} \theta_{j-m}^{(k)} b_m^{(k)} = 0\]
for 3 \(\leq\) \(k\) \(\leq\) 5 and \(j \geq 0\).  \(\tag{2.1}\)

We will solve the difference equation (2.1) to find the solution \(\theta_j^{(k)}\) for any \(j \geq 0\).

(I) The case \(k = 3\). Taking \(j = 0\) and \(j = 1\) in (2.1) yield the two initial values
\[\theta_0^{(3)} = \frac{6}{11} \quad \text{and} \quad \theta_1^{(3)} = -\theta_0^{(3)} b_1^{(3)}/b_0^{(3)} = \frac{42}{11^2}.\]
One takes \(j \geq 2\) in (2.1) and finds the equation
\[\theta_j^{(3)} b_0^{(3)} + \theta_{j-1}^{(3)} b_1^{(3)} + \theta_{j-2}^{(3)} b_2^{(3)} = 0\]
for \(j \geq 2\).
or
\[ 11\theta_j^{(3)} - 7\theta_{j-1}^{(3)} + 2\theta_{j-2}^{(3)} = 0 \quad \text{for } j \geq 2. \tag{2.2} \]

The characteristic equation \(11\lambda^2 - 7\lambda + 2 = 0\) has two roots
\[ \lambda_{3,1} = \bar{\lambda}_{3,2} = \frac{7 + i\sqrt{39}}{22}. \]

Then it is easy to obtain the solution
\[ \theta_j^{(3)} = \frac{39 - 7i\sqrt{39}}{143} \left( \frac{7 + i\sqrt{39}}{22} \right)^j + \frac{39 + 7i\sqrt{39}}{143} \left( \frac{7 - i\sqrt{39}}{22} \right)^j \quad \text{for } j \geq 0, \tag{2.3} \]
and the following decaying estimate
\[ \left| \theta_j^{(3)} \right| \leq 4\sqrt{\frac{6}{143}} \left( \sqrt{\frac{2}{11}} \right)^j \leq \frac{5}{6} \left( \frac{3}{7} \right)^j \quad \text{for } j \geq 0. \tag{2.4} \]

(II) The case \( k = 4 \)

Taking \( j = 0, 1 \) and \( j = 2 \) in (2.1) yield the initial values
\[ \theta_0^{(4)} = \frac{12}{25}, \quad \theta_1^{(4)} = \frac{12}{25} \frac{23}{25} \quad \text{and} \quad \theta_2^{(4)} = \frac{23}{25} \theta_1^{(4)} - \frac{13}{25} \theta_0^{(4)} = \frac{48}{25} \cdot 51. \tag{2.5} \]

One takes \( j \geq 3 \) in (2.1) and finds
\[ \theta_j^{(4)} b_0^{(4)} + \theta_{j-1}^{(4)} b_1^{(4)} + \theta_{j-2}^{(4)} b_2^{(4)} + \theta_{j-3}^{(4)} b_3^{(4)} = 0 \quad \text{for } j \geq 3. \tag{2.6} \]

The characteristic equation \(25\lambda^3 - 23\lambda^2 + 13\lambda - 3 = 0\) has three roots
\[ \lambda_{4,1} = \bar{\lambda}_{4,2} = \frac{23}{75} - \frac{(1 + i\sqrt{3})\nu}{75\sqrt{4}} + \frac{223(1 - i\sqrt{3})}{75\sqrt{2}\nu} \approx 0.269261 - 0.492t, \]
\[ \lambda_{4,3} = \frac{23}{75} + \frac{\sqrt{2}\nu}{75} - \frac{\sqrt{4}223}{75\nu} \approx 0.381478, \]
where \( \nu := \sqrt{1921 + 225\sqrt{511}} \) and
\[ |\lambda_{4,1}| = |\lambda_{4,2}| \approx 0.560862. \]

We have the solution
\[ \theta_j^{(4)} = d_{4,1}\lambda_{4,1}^j + d_{4,2}\lambda_{4,2}^j + d_{4,3}\lambda_{4,3}^j \quad \text{for } j \geq 0, \tag{2.7} \]
where \( d_{4,i} \) for \( i = 1, 2, 3 \) are constant determined by the following equations
\[ d_{4,1}\lambda_{4,1}^j + d_{4,2}\lambda_{4,2}^j + d_{4,3}\lambda_{4,3}^j = \theta_j^{(4)} \quad \text{for } j = 0, 1, 2. \]

Numerical computations yield
\[ d_{4,1} = d_{4,2} \approx -0.359522 + 0.405803t \quad \text{and} \quad d_{4,3} \approx 0.719044. \]
Then we can obtain the following estimate

\[ |\theta_j^{(4)}| \leq \frac{3}{2} \left( \frac{4}{7} \right)^j \text{ for } j \geq 0. \]  

\[(2.7)\]

\[|\theta_j^{(4)}| \leq 3 \left( \frac{4}{7} \right)^j \text{ for } j \geq 0. \]  

\[(2.7)\]

\[(III)\] The case \(k = 5\) Taking \(j = 0, 1, 2\) and \(j = 3\) in (2.1) yield the initial values

\[\theta_0^{(5)} = \frac{60}{137}, \quad \theta_1^{(5)} = \frac{163}{137} \theta_0^{(5)} = \frac{60 \cdot 163}{137^2}, \]

\[\theta_2^{(5)} = \frac{163}{137} \theta_1^{(5)} - \theta_0^{(5)} = \frac{60(163^2 - 1)}{137^3}, \]

\[\theta_3^{(5)} = \frac{163}{137} \theta_2^{(5)} - \theta_1^{(5)} + \frac{63}{137} \theta_0^{(5)} = \frac{9780(163^2 - 1) - 6000 \cdot 137^2}{137^4}. \]

One takes \(j \geq 4\) in (2.1) and finds

\[\theta_j^{(5)} b_0^{(5)} + \theta_{j-1}^{(5)} b_1^{(5)} + \theta_{j-2}^{(5)} b_2^{(5)} + \theta_{j-3}^{(5)} b_3^{(5)} + \theta_{j-4}^{(5)} b_4^{(5)} = 0 \text{ for } j \geq 4. \]  

\[(2.8)\]

The characteristic equation \(137 \lambda_4^2 - 163 \lambda_5^2 + 137 \lambda_5^2 - 63 \lambda_5 + 12 = 0\) has four roots

\[\lambda_{5,1} = \bar{\lambda}_{5,2} \approx 0.210044 - 0.676871, \quad \lambda_{5,3} = \bar{\lambda}_{5,4} \approx 0.384847 - 0.162121. \]

Also,

\[|\lambda_{5,1}| = |\lambda_{5,2}| \approx 0.708711 \text{ and } |\lambda_{5,3}| = |\lambda_{5,4}| \approx 0.417601. \]

We have the solution

\[\theta_j^{(5)} = \sum_{i=1}^{4} d_{5,i} \lambda_{5,i} \text{ for } j \geq 0. \]  

\[(2.9)\]

The constants \(d_{5,i}\) for \(i = 1, 2, 3, 4\) are determined by the following equations

\[\sum_{i=1}^{4} d_{5,i} \lambda_{5,i}^j = \theta_j^{(5)} \text{ for } j = 0, 1, 2, 3, \]

which yield

\[d_{5,1} = \bar{d}_{5,2} \approx 0.0365741 - 0.4507631, \quad d_{5,3} = \bar{d}_{5,4} \approx -0.0365741 + 3.27211. \]

By using the fact

\[|d_{5,1}| = |d_{5,2}| \approx 0.452244 \text{ and } |d_{5,3}| = |d_{5,4}| \approx 3.27232, \]

it is not difficult to obtain the following estimate

\[|\theta_j^{(5)}| \leq 24 \left( \frac{5}{7} \right)^j \text{ for } j \geq 0. \]  

\[(2.10)\]

This completes the proof.

We close this section by noticing that the techniques in this section can also be used to handle the case \(k = 2\) for which standard energy analysis is also applicable, see also in [10] for the analysis of variable time stepping.
2.3 Decay Estimates of the starting values

Noticing that the starting values $u_1^{(k,j)}$ have different expressions \[\text{(1.9)}\] for different step indexes $k$. We shall present the decay Estimates of the starting values by using Lemma 2.5.

Lemma 2.6 There exist positive constants $c_{1,k} > 1$ such that the starting values $u_1^{(k,j)}$ satisfy

\[
|u_1^{(k,j)}| \leq \frac{c_{1,k} \rho_k}{8} \left( \frac{k}{7} \right)^{j-k} \sum_{\ell=1}^{k-1} |\nabla_u \ell| \quad \text{for } 3 \leq k \leq 5 \text{ and } j \geq k,
\]

such that

\[
\sum_{j=k}^{n} |u_1^{(k,j)}| \leq \frac{7c_{1,k} \rho_k}{8(7-k)} \sum_{\ell=1}^{k-1} |\nabla_u \ell| \quad \text{for } 3 \leq k \leq 5 \text{ and } n \geq k,
\]

where the constants $\rho_k$ are defined in Lemma 2.5.

Proof (I) The case $k = 3$. Recalling the fact $b_j^{(3)} = 0$ for $j \geq 3$, one can derive that

\[
u_1^{(3,n)} = \begin{cases} 
\theta_0^{(3)} b_2^{(3)} \nabla u^1 + \theta_0^{(3)} b_1^{(3)} \nabla u^2, & \text{for } n = 3, \\
\theta_{n-3}^{(3)} b_2^{(3)} \nabla u^1 + (\theta_{n-3}^{(3)} b_1^{(3)} + \theta_{n-4}^{(3)} b_2^{(3)}) \nabla u^2, & \text{for } n \geq 4 
\end{cases}
\]

\[
= \begin{cases} 
\frac{1}{11} \nabla u^1 - \frac{7}{11} \nabla u^2, & \text{for } n = 3, \\
\frac{1}{3} \theta_{n-3}^{(3)} \nabla u^1 - \frac{11}{6} \theta_{n-2}^{(3)} \nabla u^2, & \text{for } n \geq 4 
\end{cases}
\]

where the difference equation \[\text{(2.2)}\] was used in the case of $n \geq 4$. So Lemma 2.5 yields

\[
|u_1^{(3,3)}| \leq \frac{1}{11} |\nabla u^1| + \frac{7}{11} |\nabla u^2|,
\]

\[
|u_1^{(3,n)}| \leq \frac{1}{3} |\theta_{n-3}^{(3)}| |\nabla u^1| + \frac{11}{6} |\theta_{n-2}^{(3)}| |\nabla u^2| 
\leq \frac{\rho_3}{4} \left( \frac{3}{7} \right)^{n-3} \left( \frac{1}{3} |\nabla u^1| + \frac{11}{14} |\nabla u^2| \right) \quad \text{for } n \geq 4.
\]

The case $k = 3$ is verified by taking $c_{1,3} = 11/7$ since

\[
|u_1^{(3,j)}| \leq \frac{\rho_3}{4} \left( \frac{3}{7} \right)^{j-3} \left( \frac{1}{3} |\nabla u^1| + \frac{11}{14} |\nabla u^2| \right) \quad \text{for } j \geq 3.
\]

(II) The case $k = 4$. It only needs to consider the general case $n \geq 6$. Since $b_j^{(4)} = 0$ for $j \geq 4$, one has

\[
u_1^{(4,n)} = \theta_{n-4}^{(4)} b_3^{(4)} \nabla u^1 + \nabla u^2 \sum_{j=4}^{n} \theta_{n-j}^{(4)} b_j^{(4)} + \nabla u^3 \sum_{j=4}^{n} \theta_{n-j}^{(4)} b_j^{(4)}
\]

\[
= \theta_{n-4}^{(4)} b_3^{(4)} \nabla u^1 + (\theta_{n-4}^{(4)} b_2^{(4)} + \theta_{n-5}^{(4)} b_3^{(4)}) \nabla u^2 - \theta_{n-3}^{(4)} b_0^{(4)} \nabla u^3 \quad \text{for } n \geq 6,
\]

\[\text{ Proof (II) (continued)}\]

\[
\sum_{j=k}^{n} |u_1^{(4,j)}| \leq \frac{7c_{1,k} \rho_k}{8(7-k)} \sum_{\ell=1}^{k-1} |\nabla u \ell| \quad \text{for } 3 \leq k \leq 5 \text{ and } n \geq k,
\]

where the constants $\rho_k$ are defined in Lemma 2.5.
where the difference equation (2.5) was used. So Lemma 2.5 yields
\[ |u^{(4,n)}| \leq \frac{\rho_4}{4} \left( \frac{n-4}{4} \left| \nabla u^1 \right| + \frac{3}{2} \left| \nabla u^2 \right| + \frac{25}{21} \left| \nabla u^3 \right| \right) \quad \text{for } n \geq 6. \]

Then the estimate for \( k = 4 \) is verified by taking the fixed cases \( n = 4 \) and \( 5 \) into account.

(iii) The case \( k = 5 \). We only consider the general case \( n \geq 8 \). Since \( b_j^{(5)} = 0 \) for \( j \geq 5 \), one has
\[ u^{(5,n)} = \sum_{\ell=1}^{4} \nabla u^\ell \sum_{j=5}^{n} \theta^{(5)}_{n-j} b_j^{(5)} \nabla u^1 + (\theta^{(5)}_{n-5} b_4^{(5)} + \theta^{(5)}_{n-6} b_3^{(5)}) \nabla u^2 + (\theta^{(5)}_{n-5} b_2^{(5)} + \theta^{(5)}_{n-6} b_3^{(5)} + \theta^{(5)}_{n-7} b_4^{(5)}) \nabla u^3 - \theta^{(5)}_{n-4} b_0^{(5)} \nabla u^4 \]
for \( n \geq 8 \), where the difference equation (2.8) was used in the last term. By using Lemma 2.5, one gets
\[ |u^{(5,n)}| \leq \frac{\rho_5}{4} \left( \frac{n-5}{5} \left| \nabla u^1 \right| + \frac{4}{3} \left| \nabla u^2 \right| + \frac{25}{6} \left| \nabla u^3 \right| + \frac{23}{14} \left| \nabla u^4 \right| \right) \quad \text{for } n \geq 8. \]
The estimate for \( k = 5 \) can be verified with a finite \( c_{1,5} \) by taking the fixed cases \( n = 5, 6 \) and 7 into account. The proof is completed.

3 Discrete energy analysis for linear reaction-diffusion

We are now ready to present the main results of this work.

3.1 Stability analysis

We first consider the dissipative case with \( \beta = \beta(x) \leq 0 \). In this case, we have the following stability result.

Theorem 3.1 The time-discrete solution \( u^n \) of the BDF-\( k \) (\( 3 \leq k \leq 5 \)) scheme (1.4) for the dissipative case \( \beta = \beta(x) \leq 0 \) satisfies
\[ \| u^n \| \leq \| u^{n-1} \| + \frac{7c_{1,k}\rho_k}{4(7-k)} \sum_{\ell=1}^{k-1} \| \nabla u^\ell \| + \frac{7\rho_k}{2(7-k)} \sum_{\ell=k}^{n} \| f^\ell \| \leq \frac{7\rho_k}{2(7-k)} \left( c_{1,k} \sum_{\ell=0}^{k-1} \| u^\ell \| + \sum_{\ell=k}^{n} \| f^\ell \| \right) \quad \text{for } n \geq k, \]
where the constants \( \rho_k \) and \( c_{1,k} \) are defined in Lemmas 2.5 and 2.6 respectively.

Proof Lemmas 2.1 and 2.4 in Appendix 2.1 imply that the DOC-\( k \) kernels are positive definite for \( 3 \leq k \leq 5 \). Under the setting \( \beta = \beta(x) \), one has
\[ -2\varepsilon \sum_{j=k}^{n} \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle \nabla u^\ell, \nabla w^j \rangle \leq 0 \quad \text{and} \quad 2 \sum_{j=k}^{n} \sum_{\ell=k}^{j} \theta^{(k)}_{j-\ell} \langle \beta u^\ell, w^j \rangle \leq 0. \]
It follows from (1.12) that
\[
\|u^n\|^2 \leq \|u^{k-1}\|^2 - 2 \sum_{j=k}^{n} \langle u^{(k,j)}, u^j \rangle + 2\tau n \sum_{j=k}^{n} \sum_{\ell=k}^{j} \|\theta_{j-\ell}^{(k)} f^\ell, u^j\|
\]
\[
\leq \|u^{k-1}\|^2 + 2 n \sum_{j=k}^{n} \|u^{(k,j)}\| \|u^j\| + 2\tau n \sum_{j=k}^{n} \sum_{\ell=k}^{j} \|\theta_{j-\ell}^{(k)} f^\ell\| \|u^j\| \quad \text{for } n \geq k. \tag{3.1}
\]

Taking some integer \( n_1 \) \((k - 1 \leq n_1 \leq n)\) such that \( \|u^{n_1}\| = \max_{k-1 \leq j \leq n} \|u^j\|\). Taking \( n := n_1 \) in the above inequality, one gets
\[
\|u^{n_1}\|^2 \leq \|u^{k-1}\| \|u^{n_1}\| + 2 \|u^{n_1}\| \sum_{j=k}^{n_1} \|u^{(k,j)}\| + 2\tau \|u^{n_1}\| \sum_{j=k}^{n_1} \sum_{\ell=k}^{j} \|\theta_{j-\ell}^{(k)} f^\ell\|
\]
and thus
\[
\|u^n\| \leq \|u^{n_1}\| \leq \|u^{k-1}\| + 2 \sum_{j=k}^{n_1} \|u^{(k,j)}\| + 2\tau \sum_{j=k}^{n_1} \sum_{\ell=k}^{j} \|\theta_{j-\ell}^{(k)} f^\ell\|
\]
\[
\leq \|u^{k-1}\| + 2 \sum_{j=k}^{n} \|u^{(k,j)}\| + 2\tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} \|\theta_{j-\ell}^{(k)} f^\ell\| \quad \text{for } n \geq k. \tag{3.2}
\]

Applying Lemma 2.5 we have \( |\theta_{j-\ell}^{(k)}| \leq \frac{\rho_k}{4} (\frac{1}{7})^{j-\ell} \) for \( 3 \leq k \leq 5 \) and then
\[
2\tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} \|\theta_{j-\ell}^{(k)} f^\ell\| \leq 2\tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} |\theta_{j-\ell}^{(k)}| \|f^\ell\| = 2\tau \sum_{\ell=k}^{n} \|f^\ell\| \|\theta_{j-\ell}^{(k)} f^\ell\|
\]
\[
\leq \frac{\rho_k}{2} \sum_{\ell=k}^{n} \sum_{\ell=k}^{j} \|f^\ell\| \|\theta_{j-\ell}^{(k)} f^\ell\| \leq \frac{7\rho_k}{2(7-k)} \sum_{\ell=k}^{n} \|f^\ell\| \quad \text{for } n \geq k. \tag{3.3}
\]

Then the claimed estimate follows by using together (3.2) and Lemma 2.6.

Next we consider the general case \(|\beta(x,t)| \leq \beta^*\). In this case, we have following stability result.

**Theorem 3.2** Consider \( 3 \leq k \leq 5 \) and the bounded coefficient \( \beta(x,t) \leq \beta^* \). If the time-step size \( \tau \leq (7-k)/(7\rho_k\beta^*) \), the time-discrete solution \( u^n \) of the BDF-k scheme (1.4) satisfies
\[
\|u^n\| \leq \frac{7\rho_k}{7-k} \exp \left( \frac{7\rho_k}{7-k}\beta^* t_{n-k} \right) \left( c_{1,k} \sum_{\ell=0}^{k-1} |u^\ell| + \sum_{\ell=k}^{n} \tau |f^\ell| \right) \quad \text{for } k \leq n \leq N.
\]

where the constants \( \rho_k \) and \( c_{1,k} \) are defined by Lemmas 2.5 and 2.6 respectively.

**Proof** By the inequality (1.12) and Theorem 3.1, we aim at bounding the third term of the right hand side of (1.12),
\[
2\tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} \theta_{j-\ell}^{(k)} \langle \beta^\ell u^\ell, u^j \rangle \leq 2\beta^* \tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} |\theta_{j-\ell}^{(k)}| \|u^\ell\| \|u^j\|. \tag{3.4}
\]
Then it is not difficult to derive from (1.12) that, for \( k \leq n \leq N \),
\[
\|u^n\|^2 \leq \|u^{k-1}\|^2 + 2 \sum_{j=k}^{n} \|u^{(k,j)}\| \|u^j\| + 2 \tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} (\beta^* \|\vartheta_{j-\ell}^{(k)}\| \|u^\ell\| + \|\vartheta_{j-\ell}^{(k)} f^\ell\|) \|u^\ell\|. \tag{3.5}
\]
Taking some integer \( n_2 \) \( (k - 1 \leq n_2 \leq n) \) such that \( \|u^{n_2}\| = \max_{k-1 \leq j \leq n} \|u^j\| \), and setting \( n := n_2 \) in the above inequality (3.5), one obtains
\[
\|u^{n_2}\| \leq \|u^{k-1}\| + 2 \sum_{j=k}^{n_2} \|u^{(k,j)}\| + 2\beta^* \tau \sum_{j=k}^{n_2} \sum_{\ell=k}^{j} \|\vartheta_{j-\ell}^{(k)}\| \|u^\ell\| \|\vartheta_{j-\ell}^{(k)} f^\ell\|,
\]
and thus
\[
\|u^n\| \leq \|u^{k-1}\| + 2 \sum_{j=k}^{n} \|u^{(k,j)}\| + 2\beta^* \tau \sum_{j=k}^{n} \sum_{\ell=k}^{j} \|\vartheta_{j-\ell}^{(k)}\| \|u^\ell\| \|\vartheta_{j-\ell}^{(k)} f^\ell\|,
\]
By applying Lemma 2.5 we have
\[
\sum_{\ell=k}^{j} \|\vartheta_{j-\ell}^{(k)}\| \leq \frac{\rho_k}{4} \sum_{\ell=k}^{j} (k/7)^{j-\ell} \leq \frac{7\rho_k}{4(7-k)} \text{ for } 3 \leq k \leq 5.
\]
Then we apply Lemma 2.6 and the estimate (3.3) to find that
\[
\|u^n\| \leq \|u^{k-1}\| + \frac{7c_1\rho_k}{4(7-k)} \sum_{\ell=1}^{k-1} \|\nabla u^\ell\| + \frac{7\rho_k\beta^*}{2(7-k)} \sum_{j=k}^{n} \tau \|u^j\| + \frac{7\rho_k}{2(7-k)} \sum_{\ell=k}^{n} \tau \|f^\ell\|
\leq \frac{7c_1\rho_k}{2(7-k)} \sum_{\ell=0}^{k-1} \|u^\ell\| + \frac{\rho_k\beta^*}{2(7-k)} \sum_{j=k}^{n} \tau \|u^j\| + \frac{\rho_k}{2(7-k)} \sum_{\ell=k}^{n} \tau \|f^\ell\|. \tag{3.6}
\]
If the time-step size \( \tau \leq \frac{7-k}{7\rho_k\beta^*} \), it follows from (3.6) that
\[
\|u^n\| \leq \frac{7c_1\rho_k}{7-k} \sum_{\ell=0}^{k-1} \|u^\ell\| + \frac{\rho_k\beta^*}{7-k} \sum_{j=k}^{n-1} \tau \|u^j\| + \frac{\rho_k}{7-k} \sum_{\ell=k}^{n} \tau \|f^\ell\| \text{ for } k \leq n \leq N.
\]
Then the claimed estimate follows by using the standard Grönwall inequality.

### 3.2 Convergence analysis

Let \( \tilde{u}^n := u(t_n, x) - u^n(x) \) for \( n \geq 0 \). Then the error equation of (1.4) reads
\[
D_k \tilde{u}^n = \varepsilon \Delta \tilde{u}^n + \beta^n \tilde{u}^n + \eta^n, \quad \text{for } k \leq n \leq N, \tag{3.7}
\]
where the local consistency error \( \eta^j = D_k u(t_j) - \partial_t u(t_j) \) for \( j \geq k \). Assume that the solution is regular in time for \( t \geq t_k \) such that
\[
|\eta^j| \leq C u \tau^k \max_{t_k \leq t \leq t_j} |\vartheta_{t-\ell}^{(k+1)}(t)| \leq C u \tau^k \text{ for } j \geq k.
\]
The stability estimate in Theorem 3.2 yields
\[ \|\tilde{u}^n\| \leq \frac{7\rho_k}{7-k} \exp\left( \frac{7\rho_k}{7-k} \beta^* t_{n-k} \right) \left( c_{1,k} \sum_{\ell=0}^{k-1} \|\tilde{u}^\ell\| + \sum_{\ell=k}^{n} \tau \|\eta^\ell\| \right) \] for \( k \leq n \leq N \).

This implies the following theorem.

**Theorem 3.3** Let \( u(t_n, x) \) and \( u^n(x) \) be the solutions of the diffusion problem (1.1) and the BDF-\( k \) scheme (1.4), respectively. If the time-step size \( \tau \leq (7-k)/(7\rho_k\beta^*) \), then the time-discrete solution \( u^n \) is convergent in the \( L^2 \) norm,
\[ \|u(t_n) - u^n\| \leq \frac{7\rho_k c_{1,k}}{7-k} \exp\left( \frac{7\rho_k\beta^* t_{n-k}}{7-k} \right) \left( \sum_{\ell=0}^{k-1} \|u(t_\ell) - u^\ell\| + C u t_{n-k}\tau^k \right) \] for \( k \leq n \leq N \), where \( \rho_k \) and \( c_{1,k} \) are defined by Lemmas 2.5 and 2.6, respectively.

4 Concluding remarks

In this work, we presented a novel discrete energy analysis for the BDF-\( k \) schemes with \( 3 \leq k \leq 5 \) by using the discrete orthogonal convolution kernels technique. Our analysis is straightforward in the sense that the standard inner product with \( u^j \) is adopted, which coincides with the classical energy approach. With this straightforward approach, less spacial regularity requirement is required for the initial data by comparing with the multiplier technique which requires stronger norm for the initial data, see the stability estimates in [3, Proposition 5.1 and Theorem 5.1].

There are several remaining issues to be handled in future works:

- The present work opens up the possibility for handling the BDF-\( k \) time-stepping methods for non-linear diffusion problems, such as phase filed models [8].

- Note that a very recent work by Akrivis et al. [2] successfully applied the multiplier technique to deal with the BDF-6 scheme. It is known that a linear multistep method is zero-stable if a perturbation in the starting values of size \( \epsilon \) causes the numerical solution over any time interval to change by no more than \( O(\epsilon) \). This is called zero-stability because it is enough to check the condition for the differential equation \( y' = 0 \). It is known that the BDF-\( k \) formulas for \( k > 6 \) are not zero-stable so they cannot be used. Note that the current analysis can only cover \( k \) up to 5, and finer analysis is needed to extend the DOC kernels technique for the BDF-6 scheme.

- Another interesting topic is to investigate the discrete energy technique for the stability and convergence of the BDF-\( k \) formula (\( 3 \leq k \leq 5 \)) with variable time-steps.

References

[1] G. Akrivis, Stability of implicit-explicit backward difference formulas for nonlinear parabolic equations, SIAM J. Numer. Anal., 53 (2015), pp. 464-484.
[2] G. Akrivis, M.H. Chen, F. Yu, Z. Zhou, The energy technique for the six-step BDF method, Math. Comp., 2021, Revised, arXiv:2007.08924.

[3] G. Akrivis, E. Katsoprinakis, Backward difference formulae: new multipliers and stability properties for parabolic equations, Math. Comp., 85 (2016), pp. 2195-2216.

[4] G. Akrivis and C. Lubich, Fully implicit, linearly implicit and implicit-explicit backward difference formulae for quasi-linear parabolic equations, Numer. Math., 131 (2015), pp. 713-735.

[5] G. Dahlquist, G-stability is equivalent to A-stability, BIT, 18 (1978), pp. 384-401.

[6] U. Grenander and G. Szegö, Toeplitz Forms and Their Applications, 2nd edition, AMS Chelsea, Providence, RI, 2001.

[7] E. Hairer and G. Wanner, Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems, Springer Series in Computational Mathematics Volume 14, Second Edition, Springer-Verlag, 2002.

[8] H.-L. Liao, T. Tang and T. Zhou, On energy stable, maximum-bound preserving, second-order BDF scheme with variable steps for the Allen-Cahn equation, SIAM J. Numer. Anal., 58(4) (2020), pp. 2294-2314.

[9] H.-L. Liao, T. Tang and T. Zhou, Positive definiteness of real quadratic forms resulting from variable-step approximations of convolution operators, arXiv:2011.13383v1, 2020.

[10] H.-L. Liao and Z. Zhang, Analysis of adaptive BDF2 scheme for diffusion equations, Math. Comp., 2020, DOI: 10.1090/mcom/3585.

[11] J. Liu, Simple and efficient ALE methods with provable temporal accuracy up to fifth order for the stokes equations on time varying domains. SIAM J. Numer. Anal., 51 (2013), pp. 743-772.

[12] C. Lubich, D. Mansour, and C. Venkataraman, Backward difference time discretization of parabolic differential equations on evolving surfaces, IMA J. Numer. Anal., 33 (2013), pp. 1365-1385.

[13] O. Nevanlinna and F. Odeh, Multiplier techniques for linear multistep methods, Numer. Funct. Anal. Optim. 3 (1981), pp. 377-423.

[14] V. Thomée, Galerkin Finite Element Methods for Parabolic Problems, Second Edition, Springer-Verlag, 2006.