Discrete gradient structures of BDF methods up to fifth-order for the phase field crystal model

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Abstract

The well-known backward difference formulas (BDF) of the third, the fourth and the fifth orders are investigated for time integration of the phase field crystal model. By building up novel discrete gradient structures of the BDF-k (k = 3, 4, 5) formulas, we establish the energy dissipation laws at the discrete levels and then obtain the priori solution estimates for the associated numerical schemes (however, we can not build any discrete energy dissipation law for the corresponding BDF-6 scheme because the BDF-6 formula itself does not have any discrete gradient structures). With the help of the discrete orthogonal convolution kernels and Young-type convolution inequalities, some concise $L^2$ norm error estimates are established via the discrete energy technique. To the best of our knowledge, this is the first time such type $L^2$ norm error estimates of non-A-stable BDF schemes are obtained for nonlinear parabolic equations. Numerical examples are presented to verify and support the theoretical analysis.

Keywords: phase field crystal model; high-order BDF method; discrete gradient structure; energy dissipation law; orthogonal convolution kernels; $L^2$ norm error estimate

AMS subject classifications. 35Q99, 65M06, 65M12

1 Introduction

This work builds on the recent discrete energy analysis [20] of the backward difference formula (BDF) schemes for linear diffusion equations. The phase field crystal (PFC) model is a class of six-order nonlinear parabolic equation, which is thermodynamically consistent [7, 8] in that the free energy of the thermodynamic model is dissipative. Consider a free energy functional of Swift-Hohenberg type [7, 8],

$$E[\Phi] = \int_{\Omega} \left( \frac{1}{4} \Phi^4 + \frac{1}{2} \Phi [ -\epsilon + (1 + \Delta)^2 ] \Phi \right) \, dx,$$

(1.1)
where \( x \in \Omega \subseteq \mathbb{R}^2 \), \( \Phi \) represents the atomistic density field and \( \epsilon \in (0, 1) \) is a parameter related to the temperature. The PFC equation is given by the \( H^{-1} \) gradient flow associated with the free energy functional \( E[\phi] \),

\[
\partial_t \Phi = \Delta \mu \quad \text{with the chemical potential} \quad \mu := \frac{\delta E}{\delta \Phi} = \Phi^3 - \epsilon \Phi + (1 + \Delta)^2 \Phi. \tag{1.2}
\]

The PFC growth model is an efficient approach to simulate crystal dynamics at the atomic scale in space while on diffusive scales in time. This model has been successfully applied to a wide variety of simulations in materials science across different time scales. Related numerical schemes for the PFC model can be found in \([6, 16–19, 28]\). We assume that \( \Phi \) is periodic over the domain \( \Omega \). By the integration by parts, one can find the volume conservation,

\[
(\Phi(t), 1) = (\Phi(t_0), 1),
\]

and the following energy dissipation law,

\[
\frac{dE}{dt} = (\frac{\delta E}{\delta \Phi}, \partial_t \Phi) = (\mu, \Delta \mu) = -\|\nabla \mu\|^2 \leq 0, \tag{1.3}
\]

where we use the \( L^2 \) inner product \((f, g) := \int_{\Omega} fg \, dx\), and the associated \( L^2 \) norm \( \|f\| := \sqrt{(f, f)} \) for all \( f, g \in L^2(\Omega) \).

Let the discrete time level \( t_k = k\tau \) with the uniform time-step \( \tau := T/N \). For any discrete time sequence \( \{v^n\}_{n=0}^N \), denote \( \nabla_{\tau} v^n := v^n - v^{n-1} \) and \( \partial_{\tau} v^n := \nabla_{\tau} v^n / \tau \). Here and hereafter, let the summation \( \sum_{j=0}^i = 0 \) if the lower index \( i \) is greater than the upper index \( j \). For a fixed index \( 3 \leq k \leq 6 \), we view the BDF-k formula as a discrete convolution summation,

\[
D_k v^n := \frac{1}{\tau} \sum_{k=1}^n b_{n-k}^{(k)} \nabla_{\tau} v^k \quad \text{for} \quad n \geq k, \tag{1.4}
\]

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

\[
\sum_{\ell=1}^k \frac{1}{\ell}(1 - \zeta)^{\ell-1} = \sum_{\ell=0}^{k-1} b_{\ell}^{(k)} \zeta^{\ell} \quad \text{for} \quad 3 \leq k \leq 6. \tag{1.5}
\]

Table 1: The BDF-k kernels \( b_j^{(k)} \) generated by (1.5)

| BDF-k | \( b_0^{(k)} \) | \( b_1^{(k)} \) | \( b_2^{(k)} \) | \( b_3^{(k)} \) | \( b_4^{(k)} \) | \( b_5^{(k)} \) |
|-------|----------------|----------------|----------------|----------------|----------------|----------------|
| \( k = 3 \) | 11/10 | -7/6 | 1/3 |
| \( k = 4 \) | 25/12 | -23/12 | 13/12 | -1/4 |
| \( k = 5 \) | 137/60 | -163/60 | 137/60 | -21/20 | 1/5 |
| \( k = 6 \) | 147/60 | -213/60 | 237/60 | -163/60 | 62/60 | -1/5 |

This work is motivated in developing high-order adaptive time-stepping strategies for the long-time simulations of coarsening dynamics. Recently, the adaptive BDF2 time-stepping scheme was investigated theoretically in \([19, 21]\) for the linear diffusion equation and PFC model (1.2), respectively. The discrete energy dissipation law and the concise \( L^2 \) norm error estimate
were established under a practical step-ratio constraint. This lower order scheme would be well suited for the fast varying solutions especially in the early coarsening process \[29\]; while high-order stable methods should be more preferable for slowly varying solutions during the long-time process approaching the steady state \[4, 14, 15, 24\]. Nonetheless, due to the lack of proper discrete energy techniques, the stability and convergence of the non-A-stable BDF-k \((k = 3, 4, 5, 6)\) schemes for nonlinear phase field models have not been well studied in the literatures.

This situation was improved recently due to the seminal work \[22\] by Lubich, Mansour and Venkataraman. They noticed that the Nevanlinna-Odeh multiplier technique \[23\] is a powerful discrete tool for the stability analysis of non-A-stable BDF-k methods. This tool was applied and explored in the numerical analysis of fully implicit, linearly and implicit-explicit BDF-k approaches for linear and nonlinear parabolic problems, see related works in \[13\] and references therein. As noticed, the multiplier technique relies on the celebrated equivalence of A-stability and G-stability for linear multi-step methods by Dahlquist \[5\]. Nonetheless, it seems that the multiplier technique is inadequate to establish the energy dissipation law and \(L^2\) norm convergence for nonlinear gradient flow problems.

Practically, the preservation of \(1.3\) at each time level, called energy dissipation law, has been proven to the fundamental requirement of numerical methods for the effective simulation of long-time coarsening dynamics \[6, 12, 16, 17, 24, 26\]. We focus on the intrinsic energy stability properties of the non-A-stable BDF-k formulas themselves, that is, some positive constants \(\sigma_{Lk}\) (the larger, the better), two nonnegative quadratic functionals \(G_k\) and \(R_k\) are sought such that the BDF-k kernels \(b_{n-j}^{(k)}\) defined in \(1.5\) satisfy the following discrete gradient structure, cf. \[4, 24\] and \[26, Section 5.6\],

\[
v_n \sum_{j=1}^{n} b_{n-j}^{(k)} v_j = G_k[v_n] - G_k[v_{n-1}] + \frac{\sigma_{Lk}}{2} v_n^2 + R_k[v_n] \quad \text{for} \ n \geq k. \tag{1.6}
\]

As shown in Theorem 2.2 that the discrete gradient structure \(1.6\) plays an important role for constructing the discrete energy dissipation laws of the corresponding BDF schemes. In this work, we achieve concise discrete gradient structures for the BDF-k formulas with the constants \(\sigma_{L3} \approx 1.979, \sigma_{L4} \approx 1.601\) and \(\sigma_{L5} \approx 0.3367\), respectively, see Lemma 2.3.

To demonstrate the practical significance of discrete gradient structures, we consider the following BDF-k implicit scheme subject to the periodic boundary conditions,

\[
D_k \phi^n = \Delta_h \mu^n \quad \text{with} \quad \mu^n = (1 + \Delta_h)^2 \phi^n + (\phi^n)^3 - \epsilon \phi^n \quad \text{for} \ k \leq n \leq N. \tag{1.7}
\]

The spatial operators are approximated by the Fourier pseudo-spectral method, as described in the next section. To avoid unnecessary technical complexity, the starting solutions \(\phi^1, \phi^2, \cdots\), \(\phi^{k-1}\) are assumed to be available and accurate enough, such as, by Runge-Kutta methods \[12\].

In the \(L^2\) norm error analysis, our main discrete tool is the discrete orthogonal convolution (DOC) kernels. For the discrete BDF-k kernels \(b_{n-j}^{(k)}\) generated by \(1.5\), the corresponding DOC-k kernels \(\theta_{n-j}^{(k)}\) are defined by \[20\]

\[
\theta_{0}^{(k)} := \frac{1}{b_{0}^{(k)}} \quad \text{and} \quad \theta_{n-j}^{(k)} := -\frac{1}{b_{0}^{(k)}} \sum_{\ell=j+1}^{n} \theta_{n-\ell}^{(k)} b_{\ell-j}^{(k)} \quad \text{for} \ j = n - 1, n - 2, \cdots, k + 1, k. \tag{1.8}
\]
It is easy to find the following discrete orthogonal convolution identity:

\[
\sum_{\ell=j}^{n} \theta_{n-\ell}^{(k)} b_{\ell-j}^{(k)} \equiv \delta_{nj} \quad \text{for any } k \leq j \leq n,
\] (1.9)

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

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

By acting the associated DOC kernels \(\theta_{n-j}^{(k)}\) on the BDF-k formula \(D_k\), we get

\[
\sum_{j=k}^{n} \theta_{n-j}^{(k)} D_k \phi^j = \frac{1}{\tau} \sum_{j=k}^{n} \theta_{n-j}^{(k)} \sum_{\ell=1}^{k-1} b_{j-\ell}^{(k)} \nabla_{\tau} \phi^\ell + \frac{1}{\tau} \sum_{j=k}^{n} \theta_{n-j}^{(k)} \sum_{\ell=k}^{j} b_{j-\ell}^{(k)} \nabla_{\tau} \phi^\ell \nabla_{\tau} \phi^j \equiv \frac{1}{\tau} \phi_{i}^{(k,n)} + \partial_{\tau} \phi^n \quad \text{for } k \leq n \leq N.
\] (1.10)

where \(\phi_{i}^{(k,n)}\) represents the starting effects on the numerical solution at the time \(t_n\),

\[
\phi_{i}^{(k,n)} := \sum_{\ell=1}^{k-1} \nabla_{\tau} \phi^\ell \sum_{j=k}^{n} \theta_{n-j}^{(k)} b_{j-\ell}^{(k)} \quad \text{for } n \geq k.
\] (1.11)

By using (1.10) and (1.11), one can act the DOC-k kernels \(\theta_{j-n}^{(k)}\) on the discrete scheme (1.7) and obtain that (replacing \(n\) by \(\ell\))

\[
\partial_{\tau} \phi^j = -\phi_{i}^{(k,j)}/\tau + \sum_{\ell=k}^{j} \theta_{j-\ell}^{(k)} \Delta h \mu^\ell \quad \text{for } j \geq k.
\] (1.12)

In section 4, the \(L^2\) norm error estimates of the BDF-k schemes (1.7) are proved via the above equivalent formulation (1.12). The standard discrete energy technique will be used with the help of some novel discrete convolution inequalities in section 3. Numerical examples are presented in the last section to support our theoretical analysis.

In summary, our contributions in this paper are two-fold:

1. Novel discrete gradient structures of the BDF-k (\(k = 3, 4, 5\)) formulas are derived such that we can build up certain discrete energy dissipation laws and obtain the priori solution estimates in the energy norm for the BDF-k time-stepping schemes (1.7). However, we cannot build any discrete energy dissipation law for the corresponding BDF-6 scheme because the BDF-6 formula itself does not have any discrete gradient structures. It provides a counterexample for the conjecture by Stuart and Humphries [26, Section 5.6].

2. By developing novel discrete convolution inequalities of Young-type, we prove the \(L^2\) norm convergence with full accuracy of the BDF-k scheme (1.7). To the best of our knowledge, this is the first time that such optimal \(L^2\) norm error estimates of high-order BDF methods are proved for a nonlinear parabolic problem.
Throughout this paper, any subscripted $C$, such as $C_u$ and $C_\phi$, denotes a generic positive constant, not necessarily the same at different occurrences; while, any subscripted $c$, such as $c_\Omega$, $c_0$, $c_1$ and so on, denotes a fixed constant. Always, the appeared constants are dependent on the given data and the solution but independent of the time steps and spatial lengths.

2 Energy dissipation law and solvability

2.1 Spatial discretization and preliminary results

For simplicity of presentation, set the spatial domain $\Omega = (0, L)^2$ and consider the uniform length $h_x = h_y = h := L/M$ in two spatial directions for an even positive integer $M$. We define the discrete grids $\Omega_h := \{x_h = (ih, jh) \mid 0 \leq i, j \leq M\}$ and $\Omega^* := \{x_h = (ih, jh) \mid 1 \leq i, j \leq M\}$. Denote the space of $L$-periodic grid functions $V_h := \{v \mid v = (v_h) \text{ is } L\text{-periodic for } x_h \in \Omega_h\}$. For any grid functions $v, w \in V_h$, define the discrete inner product $\langle v, w \rangle := h^2 \sum_{x_h \in \Omega_h} v_h w_h$, the associated $L^2$ norm $\|v\| := \sqrt{\langle v, v \rangle}$. Also, we use the $L^4$ norm $\|v\|_4 = 4^{-1/4} h^{2} \sum_{x_h \in \Omega_h} |v_h|^4$ and the maximum norm $\|v\|_\infty := \max_{x_h \in \Omega_h} |v_h|$.

For a periodic function $v(x)$ on $\bar{\Omega}$, let $P_M : L^2(\Omega) \rightarrow \mathcal{F}_M$ be the standard $L^2$ projection operator onto the space $\mathcal{F}_M$, consisting of all trigonometric polynomials of degree up to $M/2$, and $I_M : L^2(\Omega) \rightarrow \mathcal{F}_M$ be the trigonometric interpolation operator [25], that is,

$$
(P_M v)(x) = \sum_{\ell, m = -M/2}^{M/2-1} \hat{\nu}_{\ell,m} e_{\ell,m}(x), \quad (I_M v)(x) = \sum_{\ell, m = -M/2}^{M/2-1} \hat{\nu}_{\ell,m} e_{\ell,m}(x),
$$

where the complex exponential basis functions $e_{\ell,m}(x) := e^{i\nu(\ell x + my)}$ with $\nu = 2\pi/L$. The coefficients $\hat{\nu}_{\ell,m}$ refer to the standard Fourier coefficients of function $v(x)$, and the pseudospectral coefficients $\hat{\nu}_{\ell,m}$ are determined such that $(I_M v)(x_h) = v_h$.

The Fourier pseudo-spectral first and second order derivatives of $v_h$ are given by

$$
D_x v_h := \sum_{\ell, m = -M/2}^{M/2-1} (i\nu \ell) \hat{\nu}_{\ell,m} e_{\ell,m}(x_h), \quad D_x^2 v_h := \sum_{\ell, m = -M/2}^{M/2-1} (i\nu \ell)^2 \hat{\nu}_{\ell,m} e_{\ell,m}(x_h).
$$

The differentiation operators $D_y$ and $D_y^2$ can be defined in the similar fashion. In turn, we can define the discrete gradient $\nabla_h$ and Laplacian $\Delta_h$ in the point-wise sense, by

$$
\nabla_h v_h := (D_x v_h, D_y v_h)^T \quad \text{and} \quad \Delta_h v_h := \nabla_h \cdot (\nabla_h v_h) = (D_x^2 + D_y^2) v_h.
$$

For any periodic grid functions $v, w \in V_h$, it is easy to check the following discrete formulas, $\langle -\Delta_h v, w \rangle = \langle \nabla_h v, \nabla_h w \rangle$, $\langle \Delta_h^2 v, w \rangle = \langle \Delta_h v, \Delta_h w \rangle$, and $\langle \Delta_h^3 v, w \rangle = -\langle \nabla_h \Delta_h v, \nabla_h \Delta_h w \rangle$. Also, we have the following embedding inequality

$$
\|v\|_\infty \leq c_\Omega \left(\|v\| + \|\Delta_h v\| \right) \quad \text{for any } v \in V_h. \tag{2.1}
$$

For the underlying volume-conservative problem, it is convenient to define a mean-zero space $
abla_h := \{v \in V_h \mid \langle v, 1 \rangle = 0\} \subset V_h$. As usual, one can introduce a discrete version of inverse
Laplacian operator \((-\Delta_h)^{-\gamma}\). For a grid function \(v \in \tilde{V}_h\), define
\[
(-\Delta_h)^{-\gamma} v_h := \sum_{\ell, m = -M/2}^{M/2-1} (\nu^2(\ell^2 + m^2))^{-\gamma} \tilde{v}_{\ell,m} e_{\ell,m}(x_h),
\]
and an \(H^{-1}\) inner product \((v, w)_{-1} := \langle (-\Delta_h)^{-1} v, w \rangle\). The associated \(H^{-1}\) norm \(\|v\|_{-1}\) can be defined by \(\|v\|_{-1} := \sqrt{(v, v)_{-1}}\). For any functions \(v \in \tilde{V}_h\), we have the generalized Hölder inequality, \(\|v\|^2 \leq \|\nabla_h v\| \|v\|_{-1}\), and the following lemma.

**Lemma 2.1** [19, Lemma 2.1] For any grid functions \(v \in \tilde{V}_h\), it holds that
\[
\|v\|^2 \leq \frac{1}{3} \|(1 + \Delta_h)v\|^2 + \frac{3}{2} \|v\|_{-1}^2.
\]

### 2.2 Unique solvability

To focus on the numerical analysis of the BDF-\(k\) solutions, it is to assume that

- **A1.** Certain starting scheme is chosen to compute the first \((k - 1)\)-level solutions \(\phi^\ell\) for \(1 \leq \ell \leq k - 1\) such that they preserve the volume, \(\langle \phi^\ell, 1 \rangle = \langle \phi^0, 1 \rangle\) for \(1 \leq \ell \leq k - 1\).

Note that, the solution \(\phi^n\) of BDF-\(k\)-scheme \([1,7]\) preserves the volume, \(\langle \phi^n, 1 \rangle = \langle \phi^0, 1 \rangle\), for \(n \geq 1\). Actually, taking the inner product of \([1,7]\) by 1 and applying the summation by parts, one has \(\langle D_k \phi^j, 1 \rangle = \langle \Delta_h \mu^j, 1 \rangle = 0\) for \(j \geq k\). Multiplying both sides of this equality by the DOC-\(k\) kernels \(\theta_{n-j}^{(k)}\) and summing the index \(j\) from \(j = k\) to \(n\), we get
\[
\sum_{j=k}^{n} \theta_{n-j}^{(k)} \langle D_k \phi^j, 1 \rangle = 0 \quad \text{for } n \geq k.
\]

It follows from \([1.10]\) that \(\langle \nabla_x \phi^n, 1 \rangle = 0\) because the assumption **A1** implies \(\langle \phi_1^{(k,n)}, 1 \rangle = 0\). Simple induction yields the conservation law, \(\langle \phi^n, 1 \rangle = \langle \phi^0, 1 \rangle\) for \(n \geq 1\).

**Theorem 2.1** If the time-step \(\tau \leq \frac{2}{3 \epsilon b_0^{(k)}}\), the BDF-\(k\) scheme \([1,7]\) is uniquely solvable.

**Proof** For any fixed time-level indexes \(n \geq k\), we consider the following energy functional \(G\) on the space \(\tilde{V}_h^* := \{z \in \tilde{V}_h | \langle z, 1 \rangle = \langle \phi^{n-1}, 1 \rangle\}\),
\[
G[z] := \frac{1}{2\tau} \langle b_0^{(k)} (z - \phi^{n-1}) + 2L^{n-1} z - \phi^{n-1}, -1 \rangle + \frac{1}{2} \| (1 + \Delta_h) z \|^2 + \frac{1}{4} \langle z^2 - 2\epsilon z, z \rangle,
\]
where \(L^{n-1} := \sum_{\ell=1}^{n-1} b_{n-\ell}^{(k)} \nabla_x \phi^\ell\). Under the time-step constraint \(\tau \leq \frac{2}{3 \epsilon b_0^{(k)}}\), the functional \(G\) is strictly convex. Actually, for any \(\lambda \in \mathbb{R}\) and any \(\psi \in \tilde{V}_h\), one has
\[
\frac{d^2 G}{d\lambda^2} [z + \lambda \psi]_{\lambda=0} = \frac{1}{\tau} b_0^{(k)} \| \psi \|_{-1}^2 + \| (1 + \Delta_h) \psi \|^2 + 3 \| \nabla \psi \|^2 - \epsilon \| \psi \|^2.
\]
where Lemma 2.1 was applied with the setting $0 < \epsilon < 1$. Also, $G[z]$ is coercive on $\mathbb{V}_h^*$. Thus the functional $G$ has a unique minimizer, denoted by $\phi^n$, if and only if it solves the equation

$$0 = \frac{dG}{d\lambda}[z + \lambda \psi]\bigg|_{\lambda=0} = \frac{1}{\tau} \langle b_0^{(k)}(z - \phi^{n-1}) + L^{n-1} \psi, \psi \rangle_{-1} + \langle (1 + \Delta_h)^2 z + z^3 - \epsilon z, \psi \rangle_{-1}.$$

This equation holds for any $\psi \in \mathbb{V}_h$ if and only if the unique minimizer $\phi^n \in \mathbb{V}_h^*$ solves

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

which is just the BDF-$k$ scheme (1.7). It completes the proof.

### 2.3 Energy dissipation law

The positive definiteness of the BDF-$k$ kernels has been established in [20, Lemma 2.4] with the help of the Grenander-Szegö theorem [13, pp. 64–65].

**Lemma 2.2** [20, Lemma 2.4] For $3 \leq k \leq 5$, the discrete BDF-$k$ kernels $b_j^{(k)}$ defined in (1.5) are positive definite in the sense that

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

where $m_{13} = 95/48$, $m_{14} = 1.628$ and $m_{15} = 0.4776$. The minimum eigenvalue of the associated quadratic form with the BDF-$k$ kernels can be bounded from below by the constant $m_{1k}$.

This result may be adequate to show that the discrete solution of (1.7) is bounded in an energy norm. However, it is inadequate to build some discrete energy dissipation laws to simulate the continuous property (1.3) at each time level. To achieve this aim, some novel quadratic decompositions (or, discrete gradient structures according to [9, 26]) for the BDF-$k$ formulas (1.4) are given in the following lemma. Some roughly lower estimates $\sigma_{Lk} \leq m_{1k}$ are then obtained for the minimum eigenvalues of the quadratic forms with the BDF-$k$ kernels $b_j^{(k)}$.

We remark that, for the order index $k = 3, 4, 5$, the appeared functionals $\mathcal{G}_k$ and $\mathcal{R}_k$ in Lemma 2.3 always involve the consecutive $(k-1)$-tuples $(v_n, v_{n-1}, \cdots, v_{n-k+2})$ and $k$-tuples $(v_n, v_{n-1}, \cdots, v_{n-k+1})$, respectively. For the simplicity of notations, we denote

$$\mathcal{G}_k[v_n] \triangleq \mathcal{G}_k[v_n, v_{n-1}, \cdots, v_{n-k+2}], \quad \mathcal{G}_k[v_{n-1}] \triangleq \mathcal{G}_k[v_{n-1}, v_{n-2}, \cdots, v_{n-k+1}]$$

$$\mathcal{R}_k[v_n] \triangleq \mathcal{R}_k[v_n, v_{n-1}, \cdots, v_{n-k+2}, v_{n-k+1}], \quad \text{for } n \geq k.$$
Lemma 2.3 For the real sequence \( \{v_k \mid k = 0, 1, 2, \ldots, N\} \), define the difference operators
\[
\delta_1 v_n := \delta_1^1 v_n = v_n - v_{n-1} \quad \text{and} \quad \delta_1^{m+1} v_n := \delta_1^m (\delta_1 v_n) = \delta_1^m v_n - \delta_1^m v_{n-1} \quad \text{for} \quad m \geq 1.
\]
Then for the step index \( k = 3, 4 \) and \( 5 \), there exists positive constant \( \sigma_{Lk} \), nonnegative quadratic functionals \( \mathcal{G}_k \) and \( \mathcal{R}_k \) such that the BDF-\( k \) kernels \( b_j^{(k)} \) defined in (1.5) satisfy
\[
v_n \sum_{j=1}^{n} b_{n-j}^{(k)} v_j = \mathcal{G}_k[v_n] - \mathcal{G}_k[v_{n-1}] + \frac{\sigma_{Lk}}{2} v_n^2 + \mathcal{R}_k[v_n] \quad \text{for} \quad n \geq k, \tag{2.2}
\]
where positive constants \( \sigma_{Lk} \), the quadratic functionals \( \mathcal{G}_k \) and \( \mathcal{R}_k \) are given by

- for \( k = 3 \), the constant \( \sigma_{L3} := \frac{95}{48} \approx 1.979 \),
  \[
  \mathcal{G}_3[v_n] := \frac{37}{96} v_n^2 - \frac{1}{8} v_{n-1}^2 + \frac{7}{24} (\delta_1 v_n)^2 = \frac{1}{6} v_n^2 + \frac{1}{6} (\frac{7}{4} v_n - v_{n-1})^2,
  \]
  \[
  \mathcal{R}_3[v_n] := \frac{1}{6} (\delta_1^2 v_n + \frac{3}{4} v_{n-1})^2;
  \]

- for \( k = 4 \), the constant \( \sigma_{L4} := \frac{4919}{3072} \approx 1.601 \),
  \[
  \mathcal{G}_4[v_n] := \frac{3433}{6144} v_n^2 - \frac{15}{64} v_{n-1}^2 + \frac{1}{8} v_{n-2}^2 + \frac{47}{192} (\delta_1 v_n)^2 - \frac{3}{16} (\delta_1 v_{n-1})^2 + \frac{3}{16} (\delta_1^2 v_n)^2 = \frac{13627}{43008} v_n^2 + \frac{7}{24} (\frac{65}{56} v_n - v_{n-1})^2 + \frac{1}{8} (\frac{3}{2} \delta_1 v_n + v_{n-2})^2,
  \]
  \[
  \mathcal{R}_4[v_n] := \frac{1}{8} (\delta_1^3 v_n + \frac{3}{2} \delta_1 v_{n-1})^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{35}{32} v_{n-1})^2;
  \]

- for \( k = 5 \), the constant \( \sigma_{L5} := \frac{64631}{1920000} \approx 0.3367 \),
  \[
  \mathcal{G}_5[v_n] := \frac{4227769}{3840000} v_n^2 - \frac{551}{1600} v_{n-1}^2 + \frac{17}{40} v_{n-2}^2 - \frac{1}{10} v_{n-3}^2 + \frac{1607}{4800} (\delta_1 v_n)^2 \]
  \[
  - \frac{39}{80} (\delta_1 v_{n-1})^2 + \frac{2}{5} (\delta_1 v_{n-2})^2 + \frac{7}{80} (\delta_1^2 v_n)^2 - \frac{2}{5} (\delta_1^2 v_{n-1})^2 + \frac{1}{5} (\delta_1^3 v_n)^2 = \frac{1198850903}{1678080000} v_n^2 + \frac{437}{900} (\frac{493}{6992} v_n - v_{n-1})^2 \]
  \[
  + \frac{9}{40} (\frac{23}{18} \delta_1 v_n + v_{n-2})^2 + \frac{1}{10} (2 \delta_1 v_n + 2 v_{n-2} - v_{n-3})^2,
  \]
  \[
  \mathcal{R}_5[v_n] := \frac{1}{10} (\delta_1^4 v_n + 2 \delta_1^2 v_{n-1})^2 + \frac{1}{8} (\delta_1^3 v_n + \frac{23}{10} \delta_1 v_{n-1})^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{1787}{800} v_{n-1})^2.
  \]

Then the associated quadratic form of BDF-\( k \) kernels \( b_j^{(k)} \) can be bounded by
\[
2 \sum_{t=k}^{n} \sum_{j=k}^{t} b_{t-j}^{(k)} v_j \geq \sigma_{Lk} \sum_{t=k}^{n} v_t^2 \quad \text{for} \quad n \geq k.
\]
The discrete gradient structures (2.2) for the BDF-k formulas with \( k = 3, 4, 5 \) can be checked by some symbolic computation software (see the appended MATHEMATICA program Appendix_BDF345decomposition.nb) or by rather lengthy but delicate calculations (Appendix A gives a detail proof of Lemma 2.3 for interested readers). Note that the quadratic decomposition for the case of \( k = 3 \) would be optimal in the sense that the resulting minimum eigenvalue bound \( \sigma_{L3} = 95/48 \) equals the lower bound \( m_{L3} \), see Lemma 2.2. The cases of \( k = 4, 5 \) seem to be nearly optimal in the sense that \( \sigma_{L4} \) and \( \sigma_{L5} \) is very close to \( m_{L4} \) and \( m_{L5} \), respectively.

The delicate quadratic decompositions (2.2) for the non-A-stable BDF-k methods significantly update the results in [26, Theorem 5.6.3] or [9, Theorem 6.2]. They are much more sharper than the recent results in [4, Theorems 3.2 and 3.6] with the eigenvalue estimates \( \sigma_{L4} \approx 41/72 \approx 0.5694 \) and \( \sigma_{L5} = 0.1 \) for the BDF-4 and BDF-5 formulas, respectively. The present treatment gives the explicit expressions of the Lyapunov functionals \( \mathcal{G}_k \) and is quite different from the recent techniques in [4,24].

Remark 1 The BDF-6 formula might not be suited for simulating the gradient flow models, because we can not find two nonnegative quadratic functionals \( \mathcal{G}_6 \) and \( \mathcal{R}_6 \) to ensure the discrete gradient structure (2.2) for the BDF-6 formula. Otherwise, the discrete BDF-6 kernels \( b_j^{(6)} \) defined by (1.5) are at least positive semi-definite. However, it is not difficult to check that the associated quadratic form \( \sum_{m=6}^{n} v_m \sum_{j=6}^{m} b_j^{(6)} \) has negative eigenvalues. Moreover, we know that the BDF-6 formula is A(\( \alpha \))-stable with \( \alpha = 17.84^\circ \), cf. [14, Section V.2]. Thus it provides a counterexample for the conjecture by Stuart and Humphries in [26, Section 5.6], in which they inferred that the A(\( \alpha \))-stability implies the “gradient stability”.

Remark 2 Remark 4 also presents a mathematical process to explain why the \( L^2 \) norm stability (or convergence) of non-A-stable BDF time-stepping schemes (1.7) can not be done directly by multiplying with \( \phi^n \) (or the error function \( \epsilon^n = P_M \Phi^n - \phi^n \)). Actually, for the step indexes \( 3 \leq k \leq 6 \), there do not exist nonnegative quadratic functionals \( \mathcal{G}_k \) and \( \mathcal{R}_k \) such that

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

where the discrete coefficients \( d_{j}^{(k)} \) (vanish if \( j \geq k + 1 \)) are generated by

\[
\sum_{\ell=1}^{k} \frac{1}{\ell} (1 - \zeta)^\ell = \sum_{\ell=0}^{k} d_{\ell}^{(k)} \zeta^\ell \quad \text{for } k \geq 3.
\]

Otherwise, the coefficients \( d_{j}^{(k)} \) are at least positive semi-definite. Nonetheless, direct calculations show that the quadratic forms \( \sum_{m=k}^{n} v_m \sum_{j=k}^{m} d_{m-j}^{(k)} v_j \) have negative eigenvalues for \( 3 \leq k \leq 6 \). The discrete energy technique using the DOC-k kernels (1.8), described in the following sections, is an indirect approach for \( L^2 \) norm error estimates.

Let \( E[\phi^n] \) be the discrete version of free energy functional (1.1), given by

\[
E[\phi^n] := \frac{1}{2} \| (1 + \Delta_h) \phi^n \|^2 + \frac{1}{4} \| (\phi^n)^2 - \epsilon \|^2 - \frac{1}{4} \| \epsilon \|^2 \quad \text{for } n \geq 0.
\]
We define a modified discrete energy for \( n \geq k \),
\[
E_k[\phi^n] := E[\phi^n] + \frac{1}{\tau} \langle G_k[\nabla_\tau \phi^n], 1 \rangle_{-1}.
\] (2.4)

As seen, the modified discrete energy \( E_k \) introduces a perturbed term of \( O(\tau) \) to the original energy \( E[\phi^n] \) due to the application of BDF-k formula \( D_k \).

**Theorem 2.2** Assume that A1 holds and the time-step sizes are properly small such that
\[
\tau \leq \frac{2}{3\epsilon} \min \{ b_{Lk}^{(k)}, \sigma_{Lk} \} \quad \text{for} \quad n \geq k,
\] (2.5)

where \( \sigma_{L3} \approx 1.979 > b_{L0}^{(3)}, \sigma_{L4} \approx 1.601 < b_{L0}^{(4)} \) and \( \sigma_{L5} \approx 0.3367 < b_{L0}^{(5)} \). Then the BDF-k implicit scheme (1.7) preserves the following energy dissipation law
\[
E_k[\phi^n] \leq E_k[\phi^{n-1}] \quad \text{for} \quad n \geq k.
\]

**Proof** The first condition of (2.5) ensures the unique solvability in Theorem 2.1. We will establish the energy dissipation law under the second condition of (2.5). The volume conversation law implies \( \nabla_\tau \phi^n \in \bar{V}_h \) for \( n \geq 1 \). Then we make the inner product of (1.7) by \( (-\Delta_h)^{-1} \nabla_\tau \phi^n \) and obtain
\[
\langle D_k\phi^n, (-\Delta_h)^{-1} \nabla_\tau \phi^n \rangle + \langle (1 + \Delta_h)^2 \phi^n, \nabla_\tau \phi^n \rangle + \langle (\phi^n)^3 - \epsilon \phi^n, \nabla_\tau \phi^n \rangle = 0.
\] (2.6)

With the help of the summation by parts and \( 2a(a - b) = a^2 - b^2 + (a - b)^2 \), the second term at the left hand side of (2.6) gives
\[
\langle (1 + \Delta_h)^2 \phi^n, \nabla_\tau \phi^n \rangle = \frac{1}{2} \| (1 + \Delta_h)\phi^n \|^2 - \frac{1}{2} \| (1 + \Delta_h)\phi^{n-1} \|^2 + \frac{1}{2} \| (1 + \Delta_h)\nabla_\tau \phi^{n} \|^2.
\]

By using Lemma 2.3 with \( v_n := \nabla_\tau \phi^n \), the first term in (2.6) can be bounded by
\[
\langle D_k\phi^n, (-\Delta_h)^{-1} \nabla_\tau \phi^n \rangle \geq \frac{1}{\tau} \langle G_k[\nabla_\tau \phi^n], 1 \rangle_{-1} - \frac{1}{\tau} \langle G_k[\nabla_\tau \phi^{n-1}], 1 \rangle_{-1} + \frac{\sigma_{Lk}}{2\tau} \| \nabla_\tau \phi^{n} \|^2.
\]

It is easy to check the following identity
\[
4(a^3 - \epsilon a) (a - b) = (a^2 - \epsilon)^2 - (b^2 - \epsilon)^2 - 2(\epsilon - a^2) (a - b)^2 + (a^2 - b^2)^2.
\]

One can bound the third term in (2.6) by
\[
\langle (\phi^n)^3 - \epsilon \phi^n, \nabla_\tau \phi^n \rangle \geq \frac{1}{4} \| (\phi^n)^2 - \epsilon \|^2 - \frac{1}{4} \| (\phi^{n-1})^2 - \epsilon \|^2 - \frac{\epsilon}{2} \| \nabla_\tau \phi^n \|^2.
\]

By collecting the above estimates, it follows from (2.6) and the definition (2.4) that
\[
\frac{1}{2} \| (1 + \Delta_h)\nabla_\tau \phi^n \|^2 + \frac{\sigma_{Lk}}{2\tau} \| \nabla_\tau \phi^n \|^2 - \frac{\epsilon}{2} \| \nabla_\tau \phi^n \|^2 + E_k[\phi^n] \leq E_k[\phi^{n-1}]
\] (2.7)

for \( n \geq k \). Applying Lemma 2.1, one has
\[
\frac{\epsilon}{2} \| \nabla_\tau \phi^n \|^2 \leq \frac{1}{6} \| (1 + \Delta_h)\nabla_\tau \phi^n \|^2 + \frac{3\epsilon}{4} \| \nabla_\tau \phi^n \|^2 - 1.
\]
where $0 < \epsilon < 1$ has been used. Thus we can obtain that
\[
\frac{1}{3} \|(1 + \Delta h) \nabla \phi^n\|^2 + \left(\frac{\sigma_{Lk}}{2 \tau} - \frac{3\epsilon}{4}\right) \|\nabla \phi^n\|^2 + \mathcal{E}_k[\phi^n] \leq \mathcal{E}_k[\phi^{n-1}] \quad \text{for } n \geq k.
\]

Under the second condition of (2.5) or $\tau \leq \frac{3}{8} \sigma_{Lk}$, it yields the claimed result.

The two time-step constraints in (2.5) ensure the unique solvability and the energy stability are consistent since they have the same order of magnitude. But the constraint (2.5) always requires smaller step-sizes for the higher order methods. It is expected that some stabilized techniques [27] would remove the time-step restriction without sacrificing the time accuracy. However, this issue is out of our current scope (the mathematical treatments for some high-order explicit extrapolations seem non-trial) and will be reported in further studies.

To simplify the subsequent analysis, we impose a further assumption:

**A2.** Under the assumption A1 and the time-step constraint (2.5), assume that there exists a constant $c_0$ such that $\mathcal{E}_k[\phi^{k-1}] \leq c_0$, where $c_0$ may depend on the problem and the starting values, but is always independent of the spatial length $h$ and time-step size $\tau$.

**Lemma 2.4** If A2 holds, the solution of BDF-$k$ scheme (1.7) is stable in the $L^\infty$ norm,
\[
\|\phi^n\|_\infty \leq c_1 := c_\Omega \sqrt{8c_0 + 2(2 + \epsilon)^2 |\Omega_h|} \quad \text{for } n \geq k,
\]
where $c_1$ may depend on the problem and the starting values, but is always independent of the spatial length $h$, time-step size $\tau$ and the time $t_n$.

**Proof** The result follows from the proof of [19, Lemma 2.3] with the help of (2.1).

### 3 Some discrete convolution inequalities

#### 3.1 Some properties of DOC-$k$ kernels

Our error analysis is closely related to the discrete convolution form (1.12), so we need some detail properties of the DOC-$k$ kernels $\theta_j^{(k)}$ and the associated discrete convolution inequalities. At first, we have the following result.

**Lemma 3.1** [20, Lemma 2.1] The discrete kernels $b_j^{(k)}$ in (1.5) are positive (semi-)definite if and only if the associated DOC-$k$ kernels $\theta_j^{(k)}$ in (1.8) are positive (semi-)definite.

Thanks to Lemma 2.2 and Lemma 3.1, the DOC-$k$ kernels are positive definite. Moreover, we collect the decaying estimates in [20, Lemma 2.5] and obtain the following result.

**Lemma 3.2** For $3 \leq k \leq 5$, the associated DOC-$k$ kernels $\theta_j^{(k)}$ defined in (1.8) 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 $\rho_5 = 96/5$. 

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To facilitate the convergence analysis, we present some discrete convolution inequalities with respect to the DOC-k kernels $\theta_j^{(k)}$. For the BDF-k formula, consider the following matrices of order $m := n - k + 1$,

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

and

\[
B_k := B_{k,l} + B_{k,l}^T,
\]

(3.1)

where $3 \leq k \leq 5$ and the index $n \geq k$. Lemma 3.2 says that the real symmetric matrix $B_k$ is positive definite. Moreover, introduce the matrices

\[
\Theta_{k,l} := \begin{pmatrix}
  \theta_0^{(k)} & \theta_0^{(k)} & \cdots & \theta_0^{(k)} \\
  \theta_1^{(k)} & \theta_0^{(k)} & \cdots & \theta_1^{(k)} \\
  \vdots & \vdots & \ddots & \vdots \\
  \theta_{m-1}^{(k)} & \cdots & \theta_{m-2}^{(k)} & \theta_0^{(k)} \\
\end{pmatrix}_{m \times m}
\]

and

\[
\Theta_k := \Theta_{k,l} + \Theta_{k,l}^T,
\]

(3.2)

where the discrete kernels $b_j^{(k)}$ and $\theta_j^{(k)}$ are defined by (1.5) and (1.8), respectively. It follows from the discrete orthogonal identity (1.9) that

\[
\Theta_{k,l} = B_{k,l}^{-1},
\]

(3.3)

and thus

\[
\Theta_k := \Theta_{k,l} + \Theta_{k,l}^T = B_{k,l}^{-1} + (B_{k,l}^{-1})^T = (B_{k,l}^{-1})^T B_k B_{k,l}^{-1}.
\]

(3.4)

As stated in Lemma 3.2 the real symmetric matrix $\Theta_k$ is also positive definite.

### 3.2 Eigenvalue estimates

We present the following eigenvalue estimates of $B_{k,l}^T B_{k,l}$ and $\Theta_k$ for any indexes $n \geq k$.

**Lemma 3.3** There exists a positive constant $m_{2k}$ such that $\lambda_{\text{max}}(B_{k,l}^T B_{k,l}) \leq m_{2k}$ for $3 \leq k \leq 5$.

**Proof** For the matrix $B_{k,l}$ in (3.1) of any order $m$, $B_{k,l}^T B_{k,l}$ is a real symmetric matrix no more than $(2k - 1)$ diagonals. That is, each row of $B_{k,l}^T B_{k,l}$ has at most $(2k - 1)$ bounded elements computed from the BDF-k kernels $b_j^{(k)}$. The Gerschgorin’s circle theorem implies that there is a finite bound $m_{2k}$ such that $\lambda_{\text{max}}(B_{k,l}^T B_{k,l}) \leq m_{2k}$. □

To avoid possible confusions, we define the vector norm $\| \cdot \|$ by $\| u \| := \sqrt{u^T u}$ for any real vector $u$ and the associated matrix norm $\| A \| := \sqrt{\lambda_{\text{max}}(A^T A)}$.

**Lemma 3.4** The matrix $\Theta_k$ in (3.4) satisfies $\lambda_{\text{min}}(\Theta_k) \geq m_{1k}/m_{2k}$ for $3 \leq k \leq 5$.  

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Proof Lemma 2.2 says that real symmetric matrix $B_k$ is positive definite. There exists a non-singular upper triangular matrix $U$ such that $B_k = U^T U$. By using (3.4), one gets
\[ v^T \Theta_k v = v^T (B_{k,l}^{-1})^T B_k B_{k,l}^{-1} v = (UB_{k,l}^{-1} v)^T U B_{k,l}^{-1} v = \|U B_{k,l}^{-1} v\|^2. \]
Thus it follows that
\[ \|v\|^2 = \|B_{k,l} U^{-1} U B_{k,l}^{-1} v\|^2 \leq \|B_{k,l} U^{-1}\|^2 \|U B_{k,l}^{-1} v\|^2 \leq \|B_{k,l}\|^2 \|U^{-1}\|^2 \|v^T \Theta_k v = \lambda_{\max}(B_{k,l} B_{k,l}^T) \lambda_{\max}(B_{k,l}^{-1}) v^T \Theta_k v \]
Thus Lemmas 2.2 and 3.3 yield the claimed result.

Lemma 3.5 There exists a positive constant $m_{3k}$ such that $\lambda_{\max}(\Theta_k) \leq m_{3k}$ for $3 \leq k \leq 5$.

Proof The decaying properties of the DOC kernels $\theta_j^{(k)}$ determine the boundedness of the maximum eigenvalue of $(\Theta_k)_{m \times m}$. For an arbitrary order $m$, Lemma 3.2 shows that
\[ \rho_j := \sum_{\ell=1}^j |\theta_j^{(k)}| + \sum_{\ell=j}^m |\theta_j^{(k)}| \leq \rho_k \sum_{\ell=1}^j \left(\frac{k}{7}\right)^{j-\ell} + \rho_k \sum_{\ell=j}^m \left(\frac{k}{7}\right)^{\ell-j} \leq \frac{7\rho_k}{2(7-k)} \]
for $1 \leq j \leq m$. One takes $m_{3k} := \frac{7\rho_k}{2(7-k)}$ such that $\lambda_{\max}(\Theta_k) \leq \max_{1 \leq j \leq m} \rho_j < m_{3k}$ by the Gerschgorin’s circle theorem. It completes the proof.

3.3 Discrete convolution inequalities

The following lemmas describe some discrete convolution inequalities of Young-type. Here and hereafter, we always denote $\sum_{n,\ell} := \sum_{\ell=k} \sum_{j=k}^\ell$ for the simplicity of presentation.

Lemma 3.6 For any $\varepsilon > 0$, any real sequences $\{v_\ell\}_{\ell=k}^n$ and $\{w_\ell\}_{\ell=k}^n$, it holds that
\[ \sum_{\ell,j} \theta_{\ell-j}^{(k)} v_\ell v_\ell w_\ell \leq \varepsilon \sum_{\ell,j} \theta_{\ell-j}^{(k)} v_\ell v_\ell w_\ell + \frac{1}{2m_1 k} \varepsilon \sum_{\ell=k}^n (w_\ell)^2 \leq \varepsilon \sum_{\ell,j} \theta_{\ell-j}^{(k)} v_\ell v_\ell w_\ell + \frac{m_{2k}}{m_{1k}^2} \varepsilon \sum_{\ell,j} \theta_{\ell-j}^{(k)} v_\ell v_\ell w_\ell \]

Proof Let $w := (w_k, w_{k+1}, \cdots, w_n)^T$. A similar proof of [19] Lemma A.3 gives
\[ \sum_{\ell,j} \theta_{\ell-j}^{(k)} v_\ell v_\ell w_\ell \leq \varepsilon \sum_{\ell,j} \theta_{\ell-j}^{(k)} v_\ell v_\ell w_\ell + \frac{1}{2\varepsilon} w^T B_k^{-1} w \quad \text{for any } \varepsilon > 0. \tag{3.5} \]
From the proof Lemma 3.4 we have $B_k^{-1} = U^{-1}(U^{-1})^T$ and then
\[ w^T B_k^{-1} w = w^T U^{-1}(U^{-1})^T w = \|U^{-1} w\|^2 \leq \|U^{-1}\|^2 \|w\|^2 = \lambda_{\max}(B_k^{-1}) w^T w \leq \frac{1}{m_{1k}} w^T w = \frac{1}{m_{1k}} \sum_{\ell=k}^n (w_\ell)^2, \]
where Lemma 2.2 has been used. Inserting it into (3.5), we obtain the first claimed inequality. The second inequality follows immediately from Lemma 3.4 which gives the minimum eigenvalue estimate of $\Theta_k$. It completes the proof.
Lemma 3.7 For any $\varepsilon > 0$, any real sequences $\{v^\ell\}_{\ell=k}^n$ and $\{w^\ell\}_{\ell=k}^n$, it holds that
\[
\sum_{\ell,j}^n \theta_{\ell-j}^{(k)} v^j w^\ell \leq \varepsilon \sum_{\ell=k}^n (v^\ell)^2 + \frac{m_{3k}}{4m_{1k}\varepsilon} \sum_{\ell=k}^n (w^\ell)^2 \leq \varepsilon \sum_{\ell=k}^n (v^\ell)^2 + \frac{m_{2k}m_{3k}}{2m_{1k}^2} \sum_{\ell,j}^n \theta_{\ell-j}^{(k)} v^j w^\ell.
\]

Proof Taking $\varepsilon := 2\varepsilon_2/m_{3k}$ in the first inequality of Lemma 3.6 yields
\[
\sum_{\ell,j}^n \theta_{\ell-j}^{(k)} v^j w^\ell \leq \frac{2\varepsilon_2}{m_{3k}} \sum_{\ell,j}^n \theta_{\ell-j}^{(k)} v^j v^\ell + \frac{m_{3k}}{4m_{1k}\varepsilon_2} \sum_{\ell=k}^n (w^\ell)^2 \leq \varepsilon_2 \sum_{\ell=k}^n (v^\ell)^2 + \frac{m_{3k}}{4m_{1k}\varepsilon_2} \sum_{\ell=k}^n (w^\ell)^2,
\]
where Lemma 3.5 was used in the last inequality. The first inequality is verified by choosing $\varepsilon_2 := \varepsilon$, and the second one follows from Lemma 3.4 immediately.

Lemma 3.8 For any grid function $v^n \in \mathcal{V}_h$ and any constant $\varepsilon > 0$,
\[
\sum_{\ell,j}^n \theta_{\ell-j}^{(k)} \langle \Delta_h v^j, \Delta_h v^\ell \rangle \leq \varepsilon \sum_{\ell,j}^n \theta_{\ell-j}^{(k)} \langle \nabla_h \Delta_h v^j, \nabla_h \Delta_h v^\ell \rangle + \frac{8m_{2k}^2}{m_{1k}^2 \varepsilon_3} \sum_{\ell=k}^n \|v^\ell\|^2.
\]

Proof For any constant $\varepsilon_3 > 0$, we can apply the second inequality of Lemma 3.6 with $w^\ell := -\nabla_h \Delta_h v^\ell$, $v^j := \nabla_h v^j$ and $\varepsilon := m_{2k}/(m_{1k}^2 \varepsilon_3)$ and derive that
\[
2 \sum_{\ell,j}^n \theta_{\ell-j}^{(k)} \langle \Delta_h v^j, \Delta_h v^\ell \rangle \leq \frac{2m_{2k}}{m_{1k}^2 \varepsilon_3} \sum_{\ell,j}^n \theta_{\ell-j}^{(k)} \langle \nabla_h v^j, \nabla_h v^\ell \rangle + 2\varepsilon_3 \sum_{\ell,j}^n \theta_{\ell-j}^{(k)} \langle \nabla_h \Delta_h v^j, \nabla_h \Delta_h v^\ell \rangle.
\]
Similarly, by using the first inequality of Lemma 3.6 with $v^j := -\Delta_h v^j$, $w^\ell := v^\ell$ and the parameter $\varepsilon := \varepsilon_3 m_{1k}^2/(2m_{2k})$, we can get
\[
\sum_{\ell,j}^n \theta_{\ell-j}^{(k)} \langle \nabla_h v^j, \nabla_h v^\ell \rangle \leq \sum_{\ell,j}^n \theta_{\ell-j}^{(k)} \langle \Delta_h v^j, \Delta_h v^\ell \rangle + \frac{2m_{2k}}{m_{1k}^2 \varepsilon_3} \sum_{\ell=k}^n \|v^\ell\|^2.
\]
We complete the proof by summing up the above two inequalities and taking $\varepsilon_3 = \varepsilon/2$.

4 $L^2$ norm error estimate

Let $\xi^j_\Phi := D_k \Phi(t_j) - \partial_t \Phi(t_j)$ be the local consistency error of BDF-$k$ formula at the time $t = t_j$. Assume that the solution is regular in time for $t \geq t_k$ such that
\[
|\xi^j_\Phi| \leq C_\Phi \tau^k \max_{t_k \leq t \leq \tau} |\theta_{t}^{(k+1)} \Phi(t)| \leq C_\Phi \tau^k \quad \text{for } j \geq k.
\]
Then Lemma 3.2 yields
\[
\sum_{\ell=k}^{n} \tau \|\Xi^\ell\| \leq C \phi^{k+1} \sum_{\ell=k}^{n} \sum_{j=k}^{\ell} |\theta_{\ell-j}^{(k)}| \leq \frac{p_{k} t_{n-k+1}}{7-k} C \phi^{k} \text{ for } n \geq k,
\]
where the global time consistency error is defined by
\[
\Xi^\ell \equiv \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \xi_{\ell}(t_{j}) \text{ for } \ell \geq k.
\]

We use the standard semi-norms and norms in the Sobolev space \(H^m(\Omega)\) for \(m \geq 0\). Let \(C_{\text{per}}^\infty(\Omega)\) be a set of infinitely differentiable \(L\)-periodic functions defined on \(\Omega\), and \(H^m_{\text{per}}(\Omega)\) be the closure of \(C_{\text{per}}^\infty(\Omega)\) in \(H^m(\Omega)\), endowed with the semi-norm \(\|\cdot\|_{H^m_{\text{per}}}\) and the norm \(\|\cdot\|_{H^m_{\text{per}}}\).

For simplicity, denote \(|\cdot|_{H^m} := |\cdot|_{H^m_{\text{per}}}, \|\cdot\|_{H^m} := \|\cdot\|_{H^m_{\text{per}}}\), and \(\|\cdot\|_{L^2} := \|\cdot\|_{H^0}\). We denote the maximum norm by \(\|\cdot\|_{L^\infty}\) and have the Sobolev embedding inequality \(\|u\|_{L^\infty} \leq C_{\Omega} \|u\|_{H^2}\) for \(u \in C_{\text{per}}^\infty(\Omega) \cap H^m_{\text{per}}(\Omega)\). Next lemma lists some approximations, see [25], of the \(L^2\)-projection operator \(P_M\) and trigonometric interpolation operator \(I_M\) defined in subsection 2.1.

**Lemma 4.1** For any \(u \in H^q_{\text{per}}(\Omega)\) and \(0 \leq s \leq q\), it holds that
\[
\|P_M u - u\|_{H^s} \leq C u h^{q-s} |u|_{H^q}, \quad \|P_M u\|_{H^s} \leq C_u \|u\|_{H^s},
\]
and, in addition if \(q > 3/2\),
\[
\|I_M u - u\|_{H^s} \leq C u h^{q-s} |u|_{H^q}, \quad \|I_M u\|_{H^s} \leq C_u \|u\|_{H^s}.
\]

Note that, the energy dissipation law (1.3) of PFC model (1.2) shows that \(E[\Phi^n] \leq E[\Phi(t_0)]\). From the formulation (1.1), it is not difficult to see that \(\|\Phi^n\|_{H^2}\) can be bounded by a time-independent constant. By the projection estimate (4.4) in Lemma 4.1 and the Sobolev inequality, one has \(\|P_M \Phi^n\|_{L^\infty} \leq c_2\) and then
\[
\|P_M \Phi^n\|_{L^\infty} \leq \|P_M \Phi^n\|_{L^\infty} \leq c_2 \text{ for } 1 \leq n \leq N,
\]
where \(c_2\) is dependent on the domain \(\Omega\) and initial data \(\Phi(t_0)\), but independent of the time \(t_n\).

We are in the position to prove the \(L^2\) norm convergence of the BDF-k scheme (1.7) by choosing an initial value \(\phi^0 = I_M \Phi(t_0)\). In the convergence analysis, set
\[
c_3 := c_2^2 + c_1 c_2 + c_1^2 + \epsilon \quad \text{and} \quad c_4 := 250 m_2 \ell_{2k}/m_{1k}^5 + 2 c_3 m_{2k} m_{3k}/m_{1k}^2,
\]
which may be dependent on the given data, the solution and the starting values, but are always independent of the spatial length \(h\), the time-step size \(\tau\) and the time \(t_n\). Recall the following estimates on the starting values \(\phi_1^{(k,j)}\) defined in (1.11).

**Lemma 4.2** [20, Lemma 2.6] There exist some positive constants \(c_{1,k} > 1\) such that the starting values \(\phi_1^{(k,j)}\) satisfy
\[
|\phi_1^{(k,j)}| \leq \frac{c_{1,k} \rho k}{8} \left(\frac{k}{7}\right)^{j-k} \sum_{\ell=1}^{k-1} |\nabla \phi_\ell| \text{ for } 3 \leq k \leq 5 \text{ and } j \geq k,
\]
such that
\[ \sum_{j=k}^{n} |\phi^{(k,j)}_l| \leq \frac{7c_1k\rho_k}{8(7-k)} \sum_{\ell=1}^{k-1} |\nabla_{\tau}\phi^\ell| \quad \text{for } 3 \leq k \leq 5 \text{ and } n \geq k, \]
where the constants \(\rho_k\) are defined in Lemma 3.2.

**Theorem 4.1** Assume that the PFC problem \((1.2)\) has a solution \(\Phi \in C^{k+1}(0,T; H^{m+6}_{per})\) for some integer \(m \geq 0\). If \(A2\) holds and the time-step size is small such that \(\tau \leq 1/(2c_1)\), the numerical solution \(\phi^n\) of the BDF-k implicit scheme \((1.7)\) is convergent in the \(L^2\) norm,

\[ \|\Phi^n - \phi^n\| \leq \frac{7\rho_k}{\tau - k} \exp(2c_4\tau n + 1) \left( c_1k \sum_{\ell=0}^{k-1} \|\Phi^\ell_M - \phi^\ell\| + C_\phi \tau n \right), \quad k \leq n \leq N. \]

**Proof** We evaluate the \(L^2\) norm error \(\|\Phi^n - \phi^n\|\) by a usual splitting,

\[ \Phi^n - \phi^n = \Phi^n - \Phi^n_M + e^n, \]
where \(\Phi^n_M := P_M\Phi^n\) is the \(L^2\)-projection of exact solution at time \(t = t_n\) and \(e^n := \Phi^n_M - \phi^n\) is the difference between the projection \(\Phi^n_M\) and the numerical solution \(\phi^n\) of the BDF-k implicit scheme \((1.7)\). Applying Lemma 4.1 one has

\[ \|\Phi^n - \Phi^n_M\| = \|I_M(\Phi^n - \Phi^n_M)\|_{L^2} \leq C_\phi \|I_M \Phi^n - \Phi^n_M\|_{L^2} \leq C_\phi h^m \|\Phi^n\|_{H^m}. \]

Once an upper bound of \(\|e^n\|\) is available, the claimed error estimate follows immediately,

\[ \|\Phi^n - \phi^n\| \leq \|\Phi^n - \Phi^n_M\| + \|e^n\| \leq C_\phi h^m \|\Phi^n\|_{H^m} + \|e^n\| \quad \text{for } k \leq n \leq N. \quad (4.7) \]

To bound \(\|e^n\|\), we consider two stages: Stage 1 analyzes the space consistency error for a semi-discrete system having a projected solution \(\Phi_M\); With the help of the DOC-k kernels \(\theta_j^{(k)}\) and the maximum norm solution estimates in Lemma 2.4 and \((4.6)\), Stage 2 derives the error estimate from a fully discrete error system by the standard \(L^2\) norm analysis.

**Stage 1: Consistency analysis of semi-discrete projection** A substitution of the projection solution \(\Phi_M\) and differentiation operator \(\Delta_h\) into the original equation \((1.2)\) yields the semi-discrete system

\[ \partial_t \Phi_M = \Delta_h \mu_M + \zeta_P \quad \text{with} \quad \mu_M = (1 + \Delta_h)^2 \Phi_M + \left(\Phi_M\right)^3 - \epsilon \Phi_M, \quad (4.8) \]
where \(\zeta_P(x_h,t)\) represents the spatial consistency error arising from the projection of exact solution, that is,

\[ \zeta_P := \partial_t \Phi_M - \partial_t \Phi - \Delta \mu_h - \Delta_h \mu_M \quad \text{for } x_h \in \Omega_h. \quad (4.9) \]

Following the proof of [19, Theorem 3.1], and using Lemma 4.1, it is not difficult to obtain that \(\|\zeta_P\| \leq C_\phi h^m\) and \(\|\zeta_P(t_j)\| \leq C_\phi h^m\) for \(j \geq 2\). Then Lemma 3.2 yields

\[ \sum_{\ell=k}^{n} \tau \|\gamma_{\ell,j}\| \leq C_\phi \tau h^m \sum_{\ell=k}^{n} \sum_{j=k}^{\ell} |\theta_\ell^{(k)}| \leq \frac{\rho_k^2 h^{n-k+1}}{7-k} C_\phi h^m \quad \text{for } n \geq k, \quad (4.10) \]
where
\[
\Upsilon^\ell_n := \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \zeta_P(t_j) \quad \text{for } \ell \geq k. \tag{4.11}
\]

Stage 2: $L^2$ norm error of fully discrete system  From the projection equation (4.8), one can apply the BDF-k formula to obtain the following approximation equation
\[
D_k \Phi^n_M = \Delta_h \mu^n_M + \zeta^n_P + \xi^n_P \quad \text{where } \mu^n_M = (1 + \Delta_h)^2 \Phi^n_M + (\Phi^n_P)^3 - \epsilon \Phi^n_M, \tag{4.12}
\]
where $\xi^n_P$ and $\zeta^n_P := \zeta_P(t_n)$ is defined by (4.1) and (4.9), respectively. Subtracting the full discrete scheme (1.7) from the approximation equation (4.12), we have the following error system
\[
D_k e^n = \Delta_h [(1 + \Delta_h)^2 e^n + f^\ell_n e^n] + \zeta^n_P + \xi^n_P \quad \text{for } k \leq n \leq N, \tag{4.13}
\]
where $f^\ell_n := (\Phi^n_M)^2 + \Phi^n_M \phi^n + (\phi^n)^2 - \epsilon$. Thanks to the maximum norm solution estimates in Lemma 2.4 and (4.6), one has
\[
\| f^\ell_n \|_\infty \leq c_2^2 + c_1 c_2 + c_1^2 + \epsilon = c_3. \tag{4.14}
\]

Multiplying both sides of equation (4.13) by $\tau \theta_{\ell-n}^{(k)}$ and summing up $n$ from $n = k$ to $\ell$, we apply the equality (1.10) with $\nu^j = e^j$ to obtain
\[
\nabla \tau e^\ell = -e_1^{(k,\ell)} + \tau \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \Delta_h [(1 + \Delta_h)^2 e^j + f^j_n e^j] + \tau \Upsilon^\ell_P + \tau \Xi^\ell_P \quad \text{for } k \leq \ell \leq N, \tag{4.15}
\]
where $\Xi^\ell_P$ and $\Upsilon^\ell_P$ are defined by (4.3) and (4.9), respectively, and $e_1^{(k,n)}$ represents the starting error effects on the numerical solution at the time $t_n$,
\[
e_1^{(k,n)} := \sum_{\ell=1}^{k-1} \nabla \tau e^\ell \sum_{j=k}^{n} \theta_{\ell-j}^{(k)} \ell_j^{(k)} \quad \text{for } n \geq k. \tag{4.16}
\]

Making the inner product of (4.15) with $2e^\ell$, and summing up the superscript from $k$ to $n$, we have the following equality
\[
\| e^n \|^2 - \| e^{k-1} \|^2 \leq -2 \sum_{\ell=k}^{n} \langle e_1^{(k,\ell)}, e^\ell \rangle + J^n + 2\tau \sum_{\ell=k}^{n} \langle \Upsilon^\ell_P + \Xi^\ell_P, e^\ell \rangle \quad \text{for } k \leq n \leq N, \tag{4.17}
\]
where the identity $2a(a - b) = a^2 - b^2 + (a - b)^2$ is used and $J^n$ is defined by
\[
J^n := 2\tau \sum_{\ell, j}^{n, \ell} \theta_{\ell-j}^{(k)} \langle e^j + 2\Delta_h e^j + \Delta_h^2 e^j + f^j_n e^j, \Delta_h e^\ell \rangle
\]
\[
= 2\tau \sum_{\ell, j}^{n, \ell} \theta_{\ell-j}^{(k)} \left[ \langle f^j_n e^j + 2\Delta_h e^j, \Delta_h e^\ell \rangle - \langle \nabla_h e^j, \nabla_h e^\ell \rangle - \langle \nabla_h \Delta_h e^j, \nabla_h \Delta_h e^\ell \rangle \right]. \tag{4.18}
\]
Now we handle the quadratic form $J^n$. By applying the second inequality of Lemma 3.7 with $v^j := f^j_φ e^j$, $w^\ell := \Delta_h e^\ell$ and $\varepsilon = m_2 k m_3 k / m_{1k}^2$, one derives that

$$2\tau \sum_{\ell,j} n,\ell \theta^{(k)}_{\ell-j} \langle f^j_\phi e^j + 2\Delta_h e^j, \Delta_h e^\ell \rangle = 2\tau \sum_{\ell,j} n,\ell \theta^{(k)}_{\ell-j} \langle f^j_\phi e^j, \Delta_h e^\ell \rangle + 4\tau \sum_{\ell,j} n,\ell \theta^{(k)}_{\ell-j} \langle \Delta_h e^j, \Delta_h e^\ell \rangle$$

$$\leq \frac{2m_2 m_3 k}{m_{1k}^2} \sum_{\ell = k}^n \tau ||f^j_\phi e^j||^2 + 5\tau \sum_{\ell,j} n,\ell \theta^{(k)}_{\ell-j} \langle \Delta_h e^j, \Delta_h e^\ell \rangle$$

$$\leq \frac{2m_2 m_3 k}{m_{1k}^2} \sum_{\ell = k}^n \tau ||e^\ell||^2 + \frac{250m_2^2}{m_{1k}^2} \sum_{\ell = k}^n \tau ||e^\ell||^2 + 2\tau \sum_{\ell,j} n,\ell \theta^{(k)}_{\ell-j} \langle \nabla_h \Delta_h e^j, \nabla_h \Delta_h e^\ell \rangle,$$

where the maximum norm estimate (4.14), and Lemma 3.8 with $v^j := e^j$ and $\varepsilon = 2/5$ were used in the second inequality. Also, Lemma 3.2 implies that $-\sum_{\ell,j} n,\ell \theta^{(k)}_{\ell-j} \langle \nabla_h e^j, \nabla_h e^\ell \rangle \leq 0$. Then we obtain from (4.18) that

$$J^n \leq c_4 \sum_{\ell = k}^n \tau ||e^\ell||^2.$$

Therefore, it follows from (4.17) that

$$||e^n||^2 \leq ||e^{k-1}||^2 + 2 \sum_{\ell = k}^n \theta^{(k)}_{\ell} \langle ||e^\ell|| \rangle ||e^\ell|| + c_4 \sum_{\ell = k}^n \tau ||e^\ell||^2 + 2\tau \sum_{\ell = k}^n ||e^\ell|| \Upsilon_{P} + \Xi_{\Phi}^-.$$
The standard discrete Grönwall inequality yields the following estimate
\[
\|e^n\| \leq \exp\left(2c_4 t_{n-k+1} \right) \left[ \frac{\tau c_{l,k} \rho_k}{7-k} \sum_{\ell=0}^{k-1} \|e^\ell\| + 4\tau \sum_{\ell=k}^{n} (\|Y^n_\ell\| + \|\Xi^n_\ell\|) \right] \quad \text{for } k \leq n \leq N.
\]
Therefore, with the help of the error estimates (4.2) and (4.10), the triangle inequality (4.7) leads to the desired error estimate.

5 Numerical experiments

In this section, we present some numerical experiments to illustrate the efficiency of the BDF-k schemes. We notice that the proposed methods lead to nonlinear algebraic systems, which can be solved by fixed-point iterative methods with the termination error $10^{-12}$, see e.g. [10]. Due to periodic boundary conditions, the fast Fourier transform can be applied for every iteration step. The sixth-order Gaussian collocation method [11] is employed to initiate the numerical schemes such that the assumptions A1 and A2 would be reasonably fulfilled.

Example 5.1 We consider the exterior-forced PFC model $\partial_t \Phi = \Delta \mu + g(x, t)$ with the model parameter $\epsilon = 0.02$, which has an exact solution $\Phi = \cos(t) \sin(\frac{\pi}{2}x) \sin(\frac{\pi}{2}y)$.

Table 2: Numerical accuracy of BDF3 scheme.

| $N$  | $\tau$  | $\varepsilon(N)$ | Order |
|------|---------|------------------|-------|
| 10   | 1.00e-01| 1.85e-04         | –     |
| 20   | 5.00e-02| 2.42e-05         | 2.94  |
| 40   | 2.50e-02| 3.08e-06         | 2.98  |
| 80   | 1.25e-02| 3.71e-07         | 3.05  |
| 160  | 6.25e-03| 4.60e-08         | 3.01  |

Table 3: Numerical accuracy of BDF4 scheme.

| $N$  | $\tau$  | $\varepsilon(N)$ | Order |
|------|---------|------------------|-------|
| 10   | 1.00e-01| 1.19e-05         | –     |
| 20   | 5.00e-02| 7.97e-07         | 3.90  |
| 40   | 2.50e-02| 5.14e-08         | 3.95  |
| 80   | 1.25e-02| 3.26e-09         | 3.98  |
| 160  | 6.25e-03| 2.05e-10         | 4.00  |

The domain $\Omega = (0, 8)^2$ is divided into a $128 \times 128$ mesh such that the temporal error dominates the spatial error in each run. We solve the problem until time $T = 1$. The numerical results are tabulated in Tables 2-4, in which the discrete $L^2$ norm error $\varepsilon(N) := \|\Phi(T) - \phi^N\|$ is recorded in each run and the experimental order is computed by $\text{Order} \approx \log_2 (\varepsilon(N)/\varepsilon(2N))$. It is observed that the BDF-k scheme is kth-order accuracy in time.
Table 4: Numerical accuracy of BDF5 scheme.

| $N$  | $\tau$     | $e(N)$      | Order |
|------|------------|-------------|-------|
| 10   | 1.00e-01   | 3.85e-06    | –     |
| 20   | 5.00e-02   | 9.53e-08    | 5.34  |
| 40   | 2.50e-02   | 1.80e-09    | 5.72  |
| 80   | 1.25e-02   | 3.86e-11    | 5.54  |
| 160  | 6.25e-03   | 1.16e-12    | 5.06  |

Figure 1: The crystal growth process obtained at $t = 1, 200, 300, 400, 500$ and $1000$ by the BDF-5 scheme (the BDF-3 and BDF-4 schemes generate similar profiles).

Figure 2: Evolutions of original energy (left) and volume difference (right)
Example 5.2 We take the parameter \( \epsilon = 0.25 \) and use a \( 256 \times 256 \) uniform mesh to discretize the spatial domain \( \Omega = (0, 256)^2 \). As seeds for nucleation, three random perturbations on the three small square patches are taken as \( \Phi_0(\mathbf{x}) = \Phi + A \cdot \text{rand}(\mathbf{x}) \), where the constant density \( \Phi = 0.285 \), \( A \) is amplitude and the random numbers \( \text{rand}(\cdot) \) are uniformly distributed in \((-1, 1)\). The centers of three paths locate at \((64, 196)\), \((128, 64)\) and \((196, 196)\), with the corresponding amplitudes \( A = 0.25 \), \( 0.3 \) and \( 0.35 \), respectively. The length of each small square is set to 10. The solution is computed until the time \( T = 1000 \) with a constant time step \( \tau = 0.1 \).

The time evolutions of the phase variable are depicted in Figure 1. It is clear that the speed of moving interfaces is related to the initial amplitude \( A \), the larger the amplitude \( A \), the faster the crystal growth. And three different crystal grains grow and become large enough to form grain boundaries eventually. The discrete energy and the volume difference are shown in Figure 2. As predicted by our theory, the discrete volume is conservative (up to a tolerance \( 10^{-9} \)). It can be seen that the energy dissipates very fast at the early stage, and gradually slows down as the time escapes.

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A Proof of Lemma 2.3

This proof describes some quadratic decompositions of the following quantity

\[
\mathfrak{B}_k^n := v_n \sum_{j=1}^n b_{n-j}^{(k)} v_j = b_0^{(k)} v_n^2 + b_1^{(k)} v_n v_{n-1} + \cdots + b_{k-1}^{(k)} v_n v_{n-k+1} \quad \text{for } n \geq k,
\]

where the discrete BDF-k kernels \( b_j^{(k)} \) (vanish if \( j \geq k \)) are generated by (1.5), see Table 1. According to the derivations of BDF-k formulas, we use the difference operators \( \delta_1^m v_n \) to find

\[
\sum_{j=1}^n b_{n-j}^{(k)} v_j = \sum_{m=1}^k \frac{1}{m} \delta_1^{m-1} v_n = v_n + \frac{1}{2} \delta_1 v_n + \frac{1}{3} \delta_1^2 v_n + \cdots + \frac{1}{m} \delta_1^{m-1} v_n.
\]

It implies that

\[
\mathfrak{B}_k^n = \sum_{m=1}^k \frac{1}{m} v_n \delta_1^{m-1} v_n = \sum_{m=1}^k \frac{1}{2m} J_{m-1}[v_n], \quad \text{where} \quad J_m[v_n] := 2 v_n \delta_1^m v_n. \quad (A.1)
\]

Obviously, we have two trivial cases,

\[
\mathfrak{B}_1^n = \frac{1}{2} f_0[v_n] = v_n^2
\]

and

\[
\mathfrak{B}_2^n = \mathfrak{B}_1^n + \frac{1}{4} J_1[v_n] = \frac{1}{4} (v_n^2 - v_{n-1}^2) + v_n^2 + \frac{1}{4} (\delta_1 v_n)^2.
\]
In general, we will handle $J_k[v_n]$ and decompose $\mathfrak{B}^n_{k+1}$ via the following equality,

$$\mathfrak{B}^n_{k+1} = \mathfrak{B}^n_k + \frac{1}{2(k+1)} J_k[v_n] \quad \text{for } k \geq 2. \tag{A.2}$$

We prove Lemma 2.3 for the cases $k = 3, 4$ and 5 in the subsequent subsections, respectively. Our process for the quadratic decompositions includes the following three steps:

Step 1. Apply the identities $2a(a - b) = a^2 - b^2 + (a - b)^2$ and $2b(a - b) = a^2 - b^2 - (a - b)^2$ to decompose $J_m[v_n] = 2v_n\delta_1^m v_n$ in (A.1) into some quadratic terms, see (A.4), (A.9) and (A.16). Then one can obtain the preliminary (not necessarily desired) quadratic decomposition of $\mathfrak{B}^n_k$ via the recursive formula in (A.2).

Step 2. Apply the inverse decomposition formulas, see (A.5), (A.12) and (A.20), to absorb some nonpositive quadratic terms into the nonnegative terms of high-order difference. See the underlined parts in this proof, we use the nonnegative terms $(\delta_1^2 v_n + \alpha v_{n-1})^2$, $(\delta_1^2 v_n + \beta \delta_1 v_{n-1})^2$ and $(\delta_1^2 v_n + \gamma \delta_1^2 v_{n-1})^2$ to absorb the nonpositive terms $-(\delta_1 v_{n-1})^2$, $-(\delta_1^2 v_{n-1})^2$ and $-\gamma \delta_1^2 v_{n-1})^2$, respectively. Here $\alpha$, $\beta$ and $\gamma$ are constants.

Step 3. Repeat Step 2 until the preliminary quadratic decomposition in Step 1 can be reformulated into a discrete gradient structure like (1.6).

### A.1 Decomposition for the BDF-3 formula

Consider the case of $k = 2$. By noticing that

$$2v_{n-1}\delta_1^2 v_n = v_n^2 - 2v_{n-1}^2 + v_{n-2}^2 - (\delta_1 v_n)^2 - (\delta_1 v_{n-1})^2, \tag{A.3}$$

one has

$$J_2[v_n] = 2\delta_1 v_n(\delta_1^2 v_n) + 2v_{n-1}\delta_1^2 v_n = v_n^2 - 2v_{n-1}^2 + v_{n-2}^2 - 2(\delta_1 v_{n-1})^2 + (\delta_1^2 v_n)^2. \tag{A.4}$$

Then we obtain

$$\mathfrak{B}^n_3 = \mathfrak{B}^n_2 + \frac{1}{6} J_2[v_n]$$

$$= \frac{17}{12} v_n^2 - \frac{7}{12} v_{n-1}^2 + \frac{1}{6} v_{n-2}^2 + \frac{1}{4} (\delta_1 v_n)^2 - \frac{1}{4} (\delta_1 v_{n-1})^2 + \frac{1}{6} (\delta_1^2 v_n)^2 - \frac{1}{12} (\delta_1 v_{n-1})^2.$$

We treat with the last two terms (the underlined part) as follows,

$$\tilde{R}^{\alpha}_{31} := \frac{1}{6} (\delta_1^2 v_n)^2 - \frac{1}{24} (\delta_1 v_{n-1})^2$$

$$= \frac{1}{6} (\delta_1^2 v_n)^2 + \frac{1}{12} v_{n-1}^2 - \frac{1}{24} v_n^2 - \frac{1}{12} v_{n-1}^2 - \frac{1}{24} v_{n-2}^2 + \frac{1}{24} (\delta_1 v_n)^2$$

$$= \frac{1}{6} (\delta_1^2 v_n + \frac{1}{3} v_{n-1})^2 - \frac{1}{24} v_n^2 + \frac{7}{96} v_{n-1}^2 - \frac{1}{24} v_{n-2}^2 + \frac{1}{24} (\delta_1 v_n)^2,$$

where the equality (A.3) was applied inversely, that is,

$$-(\delta_1 v_{n-1})^2 = 2v_{n-1}\delta_1^2 v_n - v_n^2 + 2v_{n-1}^2 - v_{n-2}^2 + (\delta_1 v_n)^2. \tag{A.5}$$
Then we derive that
\[
\mathfrak{B}_3^n = \left[ \frac{37}{96} v_n^2 - \frac{1}{8} v_{n-1}^2 + \frac{7}{24} (\delta_1 v_n)^2 \right] - \left[ \frac{37}{96} v_{n-1}^2 - \frac{1}{8} v_{n-2}^2 + \frac{7}{24} (\delta_1 v_{n-1})^2 \right] \\
+ \frac{95}{96} v_n^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{1}{4} v_{n-1})^2.
\]

Let \( \sigma_{L3} := 95/48 \), and
\[
\mathcal{G}_3[v_n] := \frac{37}{96} v_n^2 - \frac{1}{8} v_{n-1}^2 + \frac{7}{24} (\delta_1 v_n)^2 = \frac{1}{6} v_n^2 + \frac{1}{6} (\frac{7}{4} v_n - v_{n-1})^2 \geq 0, \tag{A.6}
\]
\[
\mathcal{R}_3[v_n] := \frac{1}{6} (\delta_1^2 v_n + \frac{1}{4} v_{n-1})^2. \tag{A.7}
\]
It follows that
\[
\mathfrak{B}_3^n = \mathcal{G}_3[v_n] - \mathcal{G}_3[v_{n-1}] + \frac{\sigma_{L3}}{2} v_n^2 + \mathcal{R}_3[v_n]. \tag{A.8}
\]
It confirms the claimed decomposition \((2.2)\) for the case of \( k = 3 \).

### A.2 Decomposition for the BDF-4 formula

Consider the case of \( k = 3 \). One follows the derivations of \((A.4)\) to obtain
\[
J_3[v_n] = 2v_n \delta_1^3 v_n = J_2[\delta_1 v_n] + 2v_{n-1} \delta_1^2 v_n - J_2[v_{n-1}] \\
= -3(\delta_1 v_{n-1})^2 + 3(\delta_1 v_{n-2})^2 - 3(\delta_1^2 v_{n-1})^2 + (\delta_1^3 v_n)^2 \\
+ v_n^2 - 3v_{n-1}^2 + 3v_{n-2}^2 - v_{n-3}^2, \tag{A.9}
\]
where the equality \((A.3)\) was also used. Then using the quadratic decomposition \((A.8)\) together with \((A.6)\) and \((A.7)\) we obtain
\[
\mathfrak{B}_4^n = \mathfrak{B}_3^n + \frac{1}{8} J_3[v_n] = \mathcal{G}_3[v_n] - \mathcal{G}_3[v_{n-1}] + R_4^n, \tag{A.10}
\]
where, by combining similar terms,
\[
R_4^n := \frac{95}{96} v_n^2 + \mathcal{R}_3[v_n] + \frac{1}{8} J_3[v_n] = \frac{107}{96} v_n^2 - \frac{3}{8} v_{n-1}^2 + \frac{3}{8} v_{n-2}^2 - \frac{1}{8} v_{n-3}^2 \\
- \frac{3}{8} (\delta_1 v_{n-1})^2 + \frac{3}{8} (\delta_1 v_{n-2})^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{1}{4} v_{n-1})^2 + \frac{1}{8} (\delta_1^3 v_n)^2 - \frac{3}{8} (\delta_1^2 v_{n-1})^2.
\]
We will handle the last two terms (the underlined part). Noticing that
\[
2\delta_1 v_{n-1} (\delta_1^3 v_n) = (\delta_1 v_n)^2 - 2(\delta_1 v_{n-1})^2 + (\delta_1 v_{n-2})^2 - (\delta_1^2 v_n)^2 - (\delta_1^2 v_{n-1})^2, \tag{A.11}
\]
or, inversely,
\[
-(\delta_1^2 v_{n-1})^2 = 2\delta_1 v_{n-1} \delta_1^3 v_n - (\delta_1 v_n)^2 + 2(\delta_1 v_{n-1})^2 - (\delta_1 v_{n-2})^2 + (\delta_1^2 v_n)^2, \tag{A.12}
\]
one can derive that
\[
\tilde{R}_{41}^{n} := \frac{1}{8}(\delta_{1}^{2}v_{n})^2 - \frac{3}{16}(\delta_{1}^{2}v_{n-1})^2 \\
= \frac{1}{8}(\delta_{1}^{2}v_{n} + \frac{3}{2}\delta_{1}v_{n-1})^2 - \frac{3}{16}(\delta_{1}v_{n})^2 + \frac{3}{32}(\delta_{1}v_{n-1})^2 - \frac{3}{16}(\delta_{1}v_{n-2})^2 + \frac{3}{16}(\delta_{1}^{2}v_{n})^2.
\]
Inserting it into the above expression of \(R_{4}^{n}\), one has
\[
R_{4}^{n} = \frac{107}{96}v_{n}^2 - \frac{3}{8}v_{n-1}^2 + \frac{3}{8}v_{n-2}^2 - \frac{1}{8}v_{n-3}^2 \\
+ \frac{3}{16}(\delta_{1}^{2}v_{n})^2 - \frac{3}{16}(\delta_{1}^{2}v_{n-1})^2 - \frac{3}{8}(\delta_{1}v_{n})^2 + \frac{3}{32}(\delta_{1}v_{n-1})^2 \\
- \frac{3}{16}(\delta_{1}v_{n})^2 - \frac{9}{64}(\delta_{1}v_{n-1})^2 + \frac{3}{16}(\delta_{1}v_{n-2})^2 + \frac{1}{6}(\delta_{1}^{2}v_{n} + \frac{1}{4}v_{n-1})^2 - \frac{9}{64}(\delta_{1}v_{n-1})^2.
\]
Now we handle the last two terms (the underlined part) by applying (A.5) as follows,
\[
\tilde{R}_{42}^{n} := \frac{1}{6}(\delta_{1}^{2}v_{n} + \frac{1}{4}v_{n-1})^2 - \frac{9}{64}(\delta_{1}v_{n-1})^2 \\
= \frac{1}{6}(\delta_{1}^{2}v_{n} + \frac{35}{32}v_{n-1})^2 - \frac{9}{64}v_{n}^2 + \frac{1}{64}v_{n-1}^2 - \frac{9}{64}v_{n-2}^2 + \frac{9}{64}(\delta_{1}v_{n})^2.
\]
Inserting it into the above expression of \(R_{4}^{n}\), one gets
\[
R_{4}^{n} = \left[ \frac{355}{2048}v_{n}^2 - \frac{7}{64}v_{n-1}^2 + \frac{1}{8}v_{n-2}^2 \right] - \left[ \frac{355}{2048}v_{n-1}^2 - \frac{7}{64}v_{n-2}^2 + \frac{1}{8}v_{n-3}^2 \right] \\
- \frac{3}{64}(\delta_{1}v_{n})^2 + \frac{3}{64}(\delta_{1}v_{n-1})^2 - \frac{3}{16}(\delta_{1}v_{n-1})^2 + \frac{3}{16}(\delta_{1}v_{n-2})^2 + \frac{3}{16}(\delta_{1}^{2}v_{n})^2 \\
- \frac{3}{16}(\delta_{1}v_{n-1})^2 + \frac{4919}{6144v_{n}}^2 + \frac{1}{8}(\delta_{1}^{2}v_{n} + \frac{3}{2}\delta_{1}v_{n-1})^2 + \frac{3}{16}(\delta_{1}^{2}v_{n} + \frac{35}{32}v_{n-1})^2.
\]
Inserting it into the equality (A.10), one gets the desired decomposition
\[
\mathbb{B}_{4}^{n} = \mathcal{G}_{4}[v_{n}] - \mathcal{G}_{4}[v_{n-1}] + \frac{\sigma_{L4}}{2}v_{n}^2 + \mathcal{R}_{4}[v_{n}],
\]
where \(\sigma_{L4} = \frac{4919}{3072}\), the functionals \(\mathcal{G}_{4}\) and \(\mathcal{R}_{4}\) are defined by
\[
\mathcal{G}_{4}[v_{n}] := \frac{3433}{6144}v_{n}^2 - \frac{15}{64}v_{n-1}^2 + \frac{1}{8}v_{n-2}^2 + \frac{47}{192}(\delta_{1}v_{n})^2 - \frac{3}{16}(\delta_{1}v_{n-1})^2 + \frac{3}{16}(\delta_{1}^{2}v_{n})^2, \\
\mathcal{R}_{4}[v_{n}] := \frac{1}{8}(\delta_{1}^{2}v_{n} + \frac{3}{2}\delta_{1}v_{n-1})^2 + \frac{1}{6}(\delta_{1}^{2}v_{n} + \frac{35}{32}v_{n-1})^2.
\]
It confirms the claimed decomposition (2.2) for the case of \(k = 4\), because the quadratic functional \(\mathcal{G}_{4}\) is non-negative, that is,
\[
\mathcal{G}_{4}[v_{n}] = \frac{3433}{6144}v_{n}^2 - \frac{3}{16}v_{n}^2 - \frac{3}{64}v_{n-1}^2 + \frac{1}{8}v_{n-2}^2 + \frac{119}{192}(\delta_{1}v_{n})^2 + \frac{3}{8}v_{n-2}(\delta_{1}v_{n}) \\
= \frac{13627}{43008}v_{n}^2 + \frac{7}{24}(\frac{65}{56}v_{n} - v_{n-1})^2 + \frac{1}{8}(\frac{3}{2}\delta_{1}v_{n} + v_{n-2})^2 \geq 0.
\]
A.3 Decomposition for the BDF-5 formula

Consider the case of $k = 4$. By using (A.3) and (A.4), one has

\[ 2v_{n-1} - 3v_{n-1} + 3v_{n-2} - v_{n-3} - (\delta_1 v_n)^2 - (\delta_1 v_{n-1})^2 + 2(\delta_1 v_{n-2})^2 - (\delta_1^2 v_{n-1})^2. \]

Then we can follow the derivations of (A.9) to obtain

\[ J_4[v_n] = 2v_n \delta_1^4 v_n = J_3[\delta_1 v_n] + 2v_{n-1} \delta_1^4 v_n - J_3[v_{n-1}] \]
\[ = v_n^2 - 4v_{n-1}^2 + 6v_{n-2}^2 - 4v_{n-3}^2 + 2v_{n-4}^2 - 4(\delta_1 v_{n-1})^2 + 8(\delta_1 v_{n-2})^2 - 4(\delta_1 v_{n-3})^2 \]
\[ - 4(\delta_1^2 v_{n-1})^2 + 6(\delta_1^2 v_{n-2})^2 - 4(\delta_1^3 v_{n-1})^2 + (\delta_1^4 v_n)^2. \] (A.16)

Then using (A.13) together with (A.14) and (A.15), we obtain

\[ B_n^5 = B_4^5 + \frac{1}{10} J_4[v_n] = G_4[v_n] - G_4[v_{n-1}] + R_n^5, \] (A.17)

where, by combining similar terms,

\[ R_n^5 = \frac{4919}{6144} v_n^2 + R_4[v_n] + \frac{1}{10} J_4[v_n] = \frac{4919}{6144} v_n^2 + \frac{1}{8} (\delta_1^3 v_n + \frac{3}{2} \delta_1 v_{n-1})^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{35}{32} v_{n-1})^2 \]
\[ + \frac{1}{10} v_n^2 - \frac{2}{5} v_{n-1}^2 + \frac{3}{5} v_{n-2}^2 - \frac{2}{5} v_{n-3}^2 + \frac{1}{10} v_{n-4}^2 - \frac{2}{5} (\delta_1 v_{n-1})^2 + \frac{4}{5} (\delta_1 v_{n-2})^2 \]
\[ - \frac{2}{5} (\delta_1^2 v_{n-1})^2 - \frac{2}{5} (\delta_1 v_{n-2})^2 + \frac{3}{5} (\delta_1^2 v_{n-2})^2 - \frac{2}{5} (\delta_1^3 v_{n-1})^2 + \frac{1}{10} (\delta_1^4 v_n)^2. \] (A.18)

Noticing that

\[ 2\delta_1^2 v_{n-1}(\delta_1^4 v_n) = (\delta_1^2 v_n)^2 - 2(\delta_1 v_{n-1})^2 + (\delta_1^2 v_{n-2})^2 - (\delta_1^3 v_n)^2 - (\delta_1^3 v_{n-1})^2, \] (A.19)

or, inversely,

\[ -(\delta_1^3 v_{n-1})^2 = 2\delta_1^2 v_{n-1}(\delta_1^4 v_n) - (\delta_1^2 v_n)^2 + 2(\delta_1^2 v_{n-1})^2 - (\delta_1^2 v_{n-2})^2 + (\delta_1 v_n)^2, \] (A.20)

we handle the last two terms (the underlined part) in (A.18) as follows

\[ \bar{R}_{51}^n := \frac{1}{10} (\delta_1^4 v_n)^2 - \frac{1}{5} (\delta_1^3 v_{n-1})^2 - \frac{1}{5} (\delta_1^3 v_n)^2 \]
\[ = \frac{1}{10} (\delta_1^4 v_n + 2\delta_1^2 v_{n-1})^2 - \frac{1}{5} (\delta_1^2 v_n)^2 - \frac{1}{5} (\delta_1^2 v_{n-2})^2 + \frac{1}{5} (\delta_1^3 v_n)^2 - \frac{1}{5} (\delta_1^3 v_{n-1})^2. \]

Then it follows from (A.18) that

\[ R_n^5 = \frac{4919}{6144} v_n^2 + \frac{1}{10} v_n^2 - \frac{2}{5} v_{n-1}^2 + \frac{3}{5} v_{n-2}^2 - \frac{2}{5} v_{n-3}^2 + \frac{1}{10} v_{n-4}^2 \]
\[ - \frac{2}{5} (\delta_1 v_{n-1})^2 + \frac{4}{5} (\delta_1 v_{n-2})^2 - \frac{2}{5} (\delta_1^2 v_{n-3})^2 + \frac{2}{5} (\delta_1^2 v_{n-2})^2 \]
\[ + \frac{1}{5} (\delta_1^3 v_n)^2 - \frac{1}{5} (\delta_1^3 v_{n-1})^2 + \frac{1}{10} (\delta_1^4 v_n + 2\delta_1^2 v_{n-1})^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{35}{32} v_{n-1})^2 \]
\[ - \frac{1}{5} (\delta_1^2 v_n)^2 - \frac{3}{10} (\delta_1^3 v_{n-1})^2 + \frac{1}{8} (\delta_1^3 v_n + \frac{3}{2} \delta_1 v_{n-1})^2 - \frac{1}{10} (\delta_1^4 v_{n-1})^2. \] (A.21)
By using (A.12), we treat with the last two terms (the underlined part) by

\[ \tilde{R}_5^n := \frac{1}{8} (\delta_1^3 v_n + \frac{3}{2} \delta_1 v_{n-1})^2 - \frac{1}{10} (\delta_1^2 v_{n-1})^2 \]
\[ = \frac{1}{8} (\delta_1^3 v_n + \frac{23}{18} \delta_1 v_{n-1})^2 - \frac{1}{10} (\delta_1 v_n) - \frac{9}{50} (\delta_1 v_{n-1})^2 - \frac{1}{10} (\delta_1 v_{n-2})^2 + \frac{1}{10} (\delta_1^2 v_n)^2. \]

Inserting it into (A.21), we obtain

\[ R_5^n = \frac{4919}{6144} v_n^2 + \frac{1}{10} v_n^2 - \frac{2}{5} v_{n-1}^2 + \frac{3}{5} v_{n-2}^2 - \frac{3}{5} v_{n-3} - \frac{1}{10} v_{n-4} - \frac{1}{10} (\delta_1 v_n)^2 \]
\[ - \frac{39}{100} (\delta_1 v_{n-1})^2 + \frac{3}{5} (\delta_1 v_{n-2})^2 + \frac{2}{5} (\delta_1 v_{n-3})^2 - \frac{2}{5} (\delta_1 v_{n-3})^2 - \frac{1}{10} (\delta_1^2 v_{n-1})^2 \]
\[ - \frac{3}{10} (\delta_2^3 v_{n-1})^2 + \frac{2}{5} (\delta_2^3 v_{n-2})^2 + \frac{1}{5} (\delta_2^3 v_{n-3})^2 - \frac{1}{5} (\delta_2^3 v_{n-3})^2 + \frac{1}{10} (\delta_1^4 v_n + 2\delta_1^2 v_{n-1})^2 \]
\[ + \frac{1}{8} (\delta_1^3 v_n + \frac{23}{18} \delta_1 v_{n-1})^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{35}{18} v_{n-1})^2 - \frac{19}{100} (\delta_1 v_{n-1})^2. \]  

(A.22)

Furthermore, one can apply (A.5) to get

\[ \tilde{R}_{53}^n := \frac{1}{6} (\delta_1^2 v_n + \frac{35}{32} v_{n-1})^2 - \frac{19}{100} (\delta_1 v_{n-1})^2 \]
\[ = \frac{1}{6} (\delta_1^2 v_n + \frac{1787}{800} v_{n-1})^2 - \frac{19}{100} v_n^2 - \frac{10089}{40000} v_{n-1}^2 - \frac{19}{100} v_{n-2}^2 + \frac{19}{100} (\delta_1 v_n)^2. \]

Then we can derive from (A.22) that

\[ R_5^n = \tilde{G}_5[v_n] - \tilde{G}_5[v_{n-1}] + \frac{\sigma L_5}{2} v_n^2 + \mathcal{R}_5[v_n], \]  

(A.23)

where the constant \( \sigma L_5 := \frac{66631}{1920000} \), the functionals \( \tilde{G}_5 \) and \( \mathcal{R}_5 \) are defined by

\[ \tilde{G}_5[v_n] := \frac{21689}{40000} v_n^2 - \frac{11}{100} v_{n-1}^2 + \frac{3}{10} v_{n-2}^2 - \frac{1}{10} v_{n-3}^2 + \frac{9}{100} (\delta_1 v_n)^2 - \frac{3}{10} (\delta_1 v_{n-1})^2 \]
\[ + \frac{2}{5} (\delta_1 v_{n-2})^2 - \frac{1}{10} (\delta_1^2 v_{n-1})^2 - \frac{2}{5} (\delta_1 v_{n-1})^2 + \frac{1}{5} (\delta_1^2 v_{n-1})^2, \]
\[ \mathcal{R}_5[v_n] := \frac{1}{10} (\delta_1^4 v_n + 2\delta_1^2 v_{n-1})^2 + \frac{1}{8} (\delta_1^3 v_n + \frac{23}{18} \delta_1 v_{n-1})^2 + \frac{1}{6} (\delta_1^2 v_n + \frac{1787}{800} v_{n-1})^2. \]

Return to (A.17) and one gets claimed decomposition (2.2) for \( k = 5 \),

\[ \mathcal{B}_5^n = \tilde{G}_5[v_n] - \tilde{G}_5[v_{n-1}] + \frac{\sigma L_5}{2} v_n^2 + \mathcal{R}_5[v_n], \]  

(A.24)

where, by using (A.14),

\[ \tilde{G}_5[v_n] := G_5[v_n] + \tilde{G}_5[v_n] 
\]
\[ = \frac{4227769}{3840000} v_n^2 - \frac{551}{1600} v_{n-1}^2 + \frac{17}{40} v_{n-2}^2 - \frac{1}{10} v_{n-3}^2 + \frac{1607}{4800} (\delta_1 v_n)^2 \]
\[ - \frac{39}{80} (\delta_1 v_{n-1})^2 + \frac{2}{5} (\delta_1 v_{n-2})^2 + \frac{7}{80} (\delta_1^2 v_{n-1})^2 + \frac{2}{5} (\delta_1^2 v_{n-1})^2 + \frac{1}{5} (\delta_1^3 v_n)^2. \]  

(A.25)
By following the treatment of $\mathcal{G}_4$ in the above subsection, it is not difficult to find that
\[
\mathcal{G}_5[v_n] = \frac{1198850903}{1678080000} v_n^2 + \frac{437}{900} (\frac{4931}{6992} v_n - v_{n-1})^2
+ \frac{9}{40} (\frac{23}{18} v_n + v_{n-2})^2 + \frac{1}{10} (2\delta_1 v_n + 2v_{n-2} - v_{n-3})^2 \geq 0.
\]

The proof of Lemma 2.3 is completed.

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