WEIGHTED AND SHIFTED BDF3 METHODS ON VARIABLE GRIDS FOR A PARABOLIC PROBLEM

MINGHUA CHEN, FAN YU, QINGDONG ZHANG, AND ZHIMIN ZHANG

Abstract. As is well known, the stability of the 3-step backward differentiation formula (BDF3) on variable grids for a parabolic problem is analyzed in [Calvo and Grigorieff, BIT. 42 (2002) 689–701] under the condition $r_k := \tau_k/\tau_{k-1} < 1.199$, where $r_k$ is the adjacent time-step ratio. In this work, we establish the spectral norm inequality, which can be used to give an upper bound for the inverse matrix. Then the BDF3 scheme is unconditionally stable under a new condition $r_k \leq 1.405$. Meanwhile, we show that the upper bound of the ratio $r_k$ is less than $\sqrt{3}$ for BDF3 scheme. In addition, based on the idea of [Wang and Ruuth, J. Comput. Math. 26 (2008) 838–855; Chen, Yu, and Zhang, arXiv:2108.02910], we design a weighted and shifted BDF3 (WSBDF3) scheme for solving the parabolic problem. We prove that the WSBDF3 scheme is unconditionally stable under the condition $r_k \leq 1.771$, which is a significant improvement for the maximum time-step ratio. The error estimates are obtained by the stability inequality. Finally, numerical experiments are given to illustrate the theoretical results.

1. Introduction

Let $T > 0$, $u^0 \in H$, and consider the initial value problem of seeking $u \in C([0, T]; D(A)) \cap C([0, T]; H)$ satisfying [1, 2, 4, 16]

$$
\begin{cases}
  u'(t) + Au(t) = f(t), & 0 < t < T, \\
  u(0) = u^0
\end{cases}
$$

with $A$ a positive definite, selfadjoint, linear operator on a Hilbert space $(H, (\cdot, \cdot))$ with domain $D(A)$ dense in $H$ and $f : [0, T] \to H$ a given forcing term.

Let $N \in \mathbb{N}$ and choose the nonuniform time levels $0 = t_0 < t_1 < \cdots < t_N = T$ with the time-step $\tau_k = t_k - t_{k-1}$ for $1 \leq k \leq N$. For any time sequence $\{v^n\}_{n=0}^N$, denote

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

For $k = 1, 2, 3$, let $\Pi_{n,k} v$ denote the Lagrange interpolating polynomial of a function $v$ over $k + 1$ nodes $t_n, t_{n-1}, \ldots, t_{n-k}$. Define the adjacent time step ratio

$$
r_k := \frac{\tau_k}{\tau_{k-1}}, \quad k \geq 2.
$$

Let $v^n = v(t_n)$. The BDF3 scheme is defined by [4, 12, 19, 20]

$$
D_3 v^n = (\Pi_{n,3} v)'(t_n) = b_0^{(n)} \nabla_\tau v^n + b_1^{(n)} \nabla_\tau v^{n-1} + b_2^{(n)} \nabla_\tau v^{n-2} = \sum_{k=1}^{n} b_{n-k}^{(n)} \nabla_\tau v^k, \quad n \geq 3.
$$

2010 Mathematics Subject Classification. Primary 65L06; Secondary 65M12.

Key words and phrases. Weighted and shifted BDF3, spectral norm inequality, variable step size, stability and convergence.
Here the coefficients are computed by
\[
\begin{align*}
 b_0^{(n)} &= \frac{(1 + r_{n-1})(1 + 2r_n + r_{n-1}(1 + 4r_n + 3r_n^2))}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_{n}r_{n-1})}, \\
 b_1^{(n)} &= \frac{-r_n^2(1 + 2r_{n-1} + r_{n}r_{n-1})^2 - r_{n-1}(1 + r_{n-1})}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_{n}r_{n-1})}, \\
 b_2^{(n)} &= \frac{-r_n^2(1 + r_{n-1})(1 + r_{n}r_{n-1})^2}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_{n}r_{n-1})} \text{ with } b_j^{(n)} = 0, \ j \geq 3.
\end{align*}
\] (1.3)

Since BDF3 method needs three starting values, for concreteness, we use BDF1 scheme and BDF2 scheme, respectively, to compute the first-level solution \( u^1 \) and second-level solution \( u^2 \), namely,
\[
\begin{align*}
 D_3 v^1 &:= D_1 v^1 = \nabla x v^1 / \tau_1, \quad D_3 v^2 := D_2 v^2 = \frac{1 + 2r_2}{\tau_2(1 + r_2)} \nabla x v^2 - \frac{r_2^2}{\tau_2(1 + r_2)} \nabla x v^1.
\end{align*}
\] (1.4)

We recursively define a sequence of approximations \( u^n \) to the nodal values \( u(t^n) \) of the exact solution by BDF3 method
\[
\begin{align*}
 D_3 u^n + Au^n = f^n, \quad n \geq 1
\end{align*}
\] (1.5)

with the initial data \( u^0 = u_0 \) and the exterior force \( f^n = f(t^n) \).

The BDF3 operator (1.2) and (1.4) is regarded as a discrete convolution summation
\[
\begin{align*}
 D_3 v^n = \sum_{k=1}^{n} b_{n-k}^{(n)} \nabla x v^k, \quad n \geq 1
\end{align*}
\] (1.6)

with \( b_0^{(1)} = 1 / \tau_1, \ b_0^{(2)} = \frac{1 + 2r_2}{\tau_2(1 + r_2)}, \ b_1^{(2)} = -\frac{r_2^2}{\tau_2(1 + r_2)} \) in (1.4) and \( b_{n-k}^{(n)} \) in (1.3).

Following the approach of [6, 16], the discrete orthogonal convolution (DOC) kernels \( \{d_{n-k}^{(n)}\}_{k=1}^{n} \) for \( 1 \leq k \leq n - 1 \) are defined by
\[
\begin{align*}
 d_0^{(n)} : = \frac{1}{b_0^{(n)}} \quad \text{and} \quad d_{n-k}^{(n)} : = -\frac{1}{b_0^{(n)}} \sum_{j=k+1}^{n} d_{n-j}^{(n)} d_{j-k}^{(j)} = -d_{n-k-1}^{(n)} d_{j}^{(j+1)} + d_{n-k-2}^{(n)} d_{j}^{(j+2)}
\end{align*}
\] (1.7)

Moreover, the DOC kernels \( \{d_{n-k}^{(n)}\}_{k=1}^{n} \) satisfy the discrete orthogonal identity
\[
\begin{align*}
 \sum_{j=k}^{n} d_{n-j}^{(n)} d_{j-k}^{(j)} = \delta_{nk} \quad \text{for } 1 \leq k \leq n.
\end{align*}
\] (1.8)

It is noted that the positive semi-definiteness of BDF3 convolution kernels \( b_{n-k}^{(n)} \) and the corresponding DOC kernels \( d_{n-k}^{(n)} \) plays an important role in our numerical analysis.

For convenience, we introduce the following matrices:
\[
\begin{align*}
 B := \begin{pmatrix}
 b_0^{(1)} & b_0^{(2)} & b_0^{(3)} & \cdots & b_0^{(n)} \\
 b_1^{(1)} & b_1^{(2)} & b_1^{(3)} & \cdots & b_1^{(n)} \\
 b_2^{(1)} & b_2^{(2)} & b_2^{(3)} & \cdots & b_2^{(n)} \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 b_{n-k}^{(1)} & b_{n-k}^{(2)} & b_{n-k}^{(3)} & \cdots & b_{n-k}^{(n)} 
\end{pmatrix} \quad \text{and} \quad D := \begin{pmatrix}
 d_0^{(1)} & d_1^{(1)} & d_2^{(1)} & \cdots & d_{n-1}^{(1)} \\
 d_0^{(2)} & d_1^{(2)} & d_2^{(2)} & \cdots & d_{n-1}^{(2)} \\
 d_0^{(3)} & d_1^{(3)} & d_2^{(3)} & \cdots & d_{n-1}^{(3)} \\
 \vdots & \vdots & \vdots & \ddots & \vdots \\
 d_0^{(n)} & d_1^{(n)} & d_2^{(n)} & \cdots & d_{n-1}^{(n)} 
\end{pmatrix}
\end{align*}
\] (1.9)
where the discrete convolution kernels $b_{n-k}^{(n)}$ and the DOC kernels $\{d_{n-k}^{(n)}\}_{k=1}^{n}$ are defined in (1.6) and (1.7), respectively. It follows from the discrete orthogonal identity (1.8) that

$$D = B^{-1}. $$

We know that a upper bound is not usually available in any norm for the inverse matrix. In this work, we establish the spectral norm inequality in Lemma 5.2, which can be used to give a upper bound for the inverse matrix. Then the stability inequality is given

$$\|u^n\| \leq \|u^0\| + C \sqrt{\sum_{k=1}^{n} \tau_k \|\theta f^k + (1 - \theta) f^{k-1}\|^2} \leq \|u^0\| + C \max_{1 \leq k \leq n} \|f^k\| $$

for the solution of (4.4). In fact, the stability result (1.10) covers BDF3 method with $r_k \leq 1.405$ if $\theta = 1$ and the weighted and shifted BDF3 (WSBDF3) scheme with $r_k \leq 1.771$ if $\theta = 1/2$.

The variable time-stepping technique is powerful in capturing the multi-scale behaviors (e.g., the solution changes rapidly in certain regions of time) for a stiff partial differential equation such as the parabolic problem \[14\]. The study of variable steps BDF2 method for ODEs and PDEs has long history including some early works \[2, 8, 10, 16\] and some very recent works \[7, 16, 6\]. As for variable steps BDF3 method for ODEs, Grigorieff et al. proved that it is zero-stable if the adjacent time-step ratio $r_k < 1.08$ in \[11\] and extended to $r_k < 1.292$ in \[12\], $r_k < 1.462$ in \[3\]. Based on the theory of the spectral radius approach, Guglielmi and Zennaro proved the zero-stability of variable steps BDF3 for $r_k < 1.501$ in \[13\]. Variable steps implicit-explicit BDF3 method is presented by Wang and Ruuth \[20\], where the zero-stability with $r_k < 1.501$ is also proved for ODEs. The stability of the variable 3-step BDF for a parabolic problem is derived by Calvo and Grigorieff \[4\] under the time-step ratio $r_k \leq 1.199$. However, it contains a prefactor of the form $\exp(CT_n)$ with $\Gamma_n = \sum_{k=2}^{n} |r_k - r_{k-1}|$, the quantity $\Gamma_n$ may be unbounded at vanishing step sizes for certain choices of time-steps. We are unaware of any other published works on the stability analysis of the variable 3-step BDF for a time-dependent PDEs.

2. Upper bound estimate for fixed adjacent time-step ratio

It is noted that the positive semi-definiteness of BDF3 convolution kernels $b_{n-k}^{(n)}$ (1.9) plays an important role in our numerical analysis. In this section, we show that the upper bound of the ratio $r_k$ is less than $\sqrt{3}$ for BDF3 scheme in a sense of the positive semi-definiteness, which will be guided to prove the unconditional stability of the variable 3-step BDF under the time-step ratio $r_k \leq 1.405$ for the parabolic problem. First, we give some lemmas that will be used later.

**Proposition 2.1.** \[17, p.28\] A matrix $P \in \mathbb{R}^{n \times n}$ is said to be positive definite in $\mathbb{R}^n$ if $(Px, x) > 0$, $\forall x \in \mathbb{R}^n$, $x \neq 0$. A real matrix $P$ of order $n$ is positive definite if and only if its symmetric part $H = \frac{P + PT}{2}$ is positive definite.
Definition 2.1. [5, p. 13] Let $n \times n$ Toeplitz matrix $T_n$ be of the following form

\[
T_n = \begin{bmatrix}
t_0 & t_{-1} & \cdots & t_{2-n} & t_{1-n} \\
t_1 & t_0 & \cdots & t_{2-n} & t_{1-n} \\
\vdots & t_1 & t_0 & \ddots & \vdots \\
t_{n-2} & \cdots & \cdots & t_1 & t_0 \\
t_{n-1} & t_{n-2} & \cdots & t_1 & t_0 
\end{bmatrix};
\]

i.e., $t_{i,j} = t_{i-j}$ and $T_n$ is constant along its diagonals. Assume that the diagonals $\{t_k\}_{k=-n+1}^{n-1}$ are the Fourier coefficients of a function $g$, i.e.,

\[
t_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(x)e^{-ikx} \, dx.
\]

Then the function $g(x) = \sum_{k=-n+1}^{n-1} t_k e^{ikx}$ is called the generating function of $T_n$.

Lemma 2.1. [5, p. 13-15] (Grenander-Szegö theorem) Let $T_n$ be given by above matrix with a generating function $g$, where $g$ is a $2\pi$-periodic continuous real-valued functions defined on $[-\pi, \pi]$. Let $\lambda_{\min}(T_n)$ and $\lambda_{\max}(T_n)$ denote the smallest and largest eigenvalues of $T_n$, respectively. Then we have

\[
g_{\min} \leq \lambda_{\min}(T_n) \leq \lambda_{\max}(T_n) \leq g_{\max},
\]

where $g_{\min}$ and $g_{\max}$ is the minimum and maximum values of $g(x)$, respectively. Moreover, if $g_{\min} < g_{\max}$, then all eigenvalues of $T_n$ satisfies

\[
g_{\min} < \lambda(T_n) < g_{\max},
\]

for all $n > 0$. In particular, if $g_{\min} > 0$, then $T_n$ is positive definite.

Lemma 2.2. [17, p. 29] (Sylvester criterion) Let $P \in \mathbb{R}^{n \times n}$ be symmetric. Then, $P$ is positive definite if and only if the dominant principal minors of $P$ are all positive.

Lemma 2.3. Let $n \times n$ matrices $K_{n \times n}$ and $L_{n \times n}$ with $p_j \neq 0$ be of the following form

\[
K_{n \times n} = \begin{pmatrix}
a_1 & b_2 & c_3 & \cdots & \\
b_2 & a_2 & b_3 & \cdots & \\
c_3 & b_3 & a_3 & \cdots & \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_n & b_n & a_n
\end{pmatrix}
\quad \text{and} \quad
L_{n \times n} = \begin{pmatrix}
p_1 & q_2 & c_3 & \cdots & \\
p_2 & q_3 & \vdots & \ddots & \\
p_3 & \vdots & \ddots & \cdots & p_n \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
p_{n-1} & q_n & \cdots & \cdots & p_n
\end{pmatrix}.
\]

Then the dominant principal minors of $K$ are

\[
\det K_{j \times j} = \det L_{j \times j}
\]

with

\[
p_1 = a_1, \quad q_2 = b_2, \quad p_2 = a_2 - \frac{1}{p_1}q_2^2,
\]

\[
q_j = b_j - \frac{q_{j-1}}{p_{j-2}}c_j \quad \text{and} \quad p_j = a_j - \frac{1}{p_{j-2}}q_j^2 - \frac{1}{p_{j-1}}q_{j-1}^2, \quad j \geq 3.
\]

Proof. Using the elementary row operations, the desired result is obtained. \qed
2.1. Ratio estimate by Grenander-Szegö theorem. Let the diagonal matrix be
\[ \Lambda = \text{diag} (\tau_1, \tau_2, \ldots, \tau_n). \]
From (1.9), we have
\[ A := \Lambda^{1/2} B \Lambda^{1/2} = \begin{pmatrix} a_0^{(1)} & a_1^{(2)} & a_2^{(3)} & \cdots & a_n^{(n)} \\ a_1^{(2)} & a_0^{(1)} & a_1^{(2)} & \cdots & a_n^{(n)} \\ a_2^{(3)} & a_1^{(2)} & a_0^{(1)} & \cdots & a_n^{(n)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_n^{(n)} & a_{n-1}^{(n)} & a_{n-2}^{(n)} & \cdots & a_0^{(1)} \end{pmatrix}. \]
Here the coefficients are computed by
\[
\begin{align*}
    a_0^{(1)} &= 1, \quad a_0^{(2)} = \frac{1 + 2r_2}{1 + r_2}, \quad a_1^{(2)} = -\frac{r_2^3}{1 + r_2}, \\
    a_0^{(n)} &= \frac{(1 + r_{n-1})[1 + 2r_n + r_{n-1}(1 + 4r_n + 3r_n^2)]}{(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\
    a_1^{(n)} &= -\frac{r_n^{3/2}[(1 + 2r_{n-1} + r_n r_{n-1})^2 - r_{n-1}(1 + r_{n-1})]}{(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\
    a_2^{(n)} &= \frac{r_n^{3/2} r_{n-1}^{5/2}(1 + r_n)^2}{(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})} \forall n \geq 3.
\end{align*}
\]
We next estimate the upper adjacent time-step ratio in a sense of \( r_{k-1} \equiv r_k \).

**Lemma 2.4.** Let (constant) adjacent time-step ratio satisfy \( r_k \leq r_{\text{max}} = 1.716, k \geq 2 \). Then the matrix \( A \) or \( B \) in (2.2) is positive semi-definite.

**Proof.** Let \( y = r_k \leq r_{\text{max}} = 1.716 \). We prove the desired result in the following two cases.

Case I: \( r_k \leq 1 \). Since
\[
2a_0^{(1)} - |a_1^{(2)}| - |a_2^{(3)}| \geq 2 - 1 - 1/3 = 2/3,
\]
and
\[
2a_0^{(2)} - |a_1^{(2)}| - |a_1^{(3)}| - |a_2^{(3)}| = -\frac{1}{(1+y)(1+y+y^2)} g(y)
\]
with
\[
g(y) = 2(1+2y)(1+y+y^2) - y^{3/2}(1+y+y^2) - y^{3/2}[(1+y)^3 - y] - y^4 - y^5 \\
\geq 2(1+2y)(1+y+y^2) - y(1+y+y^2) - y[(1+y)^3 - y] - y^4 - y^5 \\
= 2 + 4y + 3y^2 - 2y^4 - y^5 \geq 2.
\]
Moreover, we have
\[
2a_0^{(n)} - 2|a_1^{(n)}| - 2|a_2^{(n)}| = -\frac{2}{(1+y)(1+y+y^2)} g_1(y) \forall n \geq 3
\]
with
\[
g_1(y) = (1+y)^3 + y^2 + 2y^3 - y^{3/2}(1+y)^3 + y^{5/2} - y^4 - y^5 \geq (1+y)^3(1-y) + y^2 \geq 1.
\]
From the above inequalities, we know that the symmetric matrix \( A + A^T \) in (2.2) is a diagonally dominant matrix. Using the Gerschgorin circle theorem, the eigenvalues of
$A+A^T$ are greater than zero, it implies that the matrix $A$ is positive definite by Proposition 2.1. 

Case II: $1 < r_k \leq r_{\max} = 1.716$. For any real sequence $\{w_k\}_{k=1}^n$, it holds that

$$2\omega_k \sum_{j=1}^k a_{k-j}^{(k)} w_j = 2 a_0^{(k)} \omega_k^2 + 2 a_1^{(k)} \omega_k \omega_{k-1} + 2 a_2^{(k)} \omega_k \omega_{k-2}$$

$$= a_2^{(k)} \omega_k^2 + a_2^{(k)} \left( a_1^{(k)} \frac{\omega_k + \omega_{k-1}}{2a_2^{(k)}} \right)^2 - a_2^{(k)} \omega_{k-1}^2 - a_2^{(k)} \left( a_1^{(k)} \frac{\omega_k + \omega_{k-1}}{2a_2^{(k)}} \right)^2$$

$$+ 2 \left( a_0^{(k)} - a_2^{(k)} - \frac{(a_1^{(k)})^2}{2a_2^{(k)}} \right) \omega_k^2 + a_2^{(k)} \left( \omega_k + \frac{a_1^{(k)}}{2a_2^{(k)}} \omega_{k-1} + \omega_{k-2} \right)^2$$

with

$$a_0^{(k)} = a_0^{(3)}, a_1^{(k)} = a_1^{(3)}, a_2^{(k)} = a_2^{(3)}, k \geq 3.$$ 

We can check that

$$(2.4) \quad a_0^{(k)} - a_2^{(k)} - \frac{(a_1^{(k)})^2}{2a_2^{(k)}} = \frac{y^3}{8a_2^{(k)}(1+y)^2(1+y+y^2)^2} l(y) > 0 \text{ with } 1 \leq y \leq 1.731 < \sqrt{3},$$

since

$$l(y) = -8y^7 - 17y^6 + 10y^5 + 43y^4 + 42y^3 + 22y^2 + 4y - 1 \geq (10y^4 - 8r_{\max}^2y^3 - 17r_{\max}^2y^3 + 43y^3 + 42y^2 + 22y + 3) > 0.$$ 

Using (2.3) and the above equations, there exists

$$2 \sum_{k=1}^n \sum_{j=1}^k b_{\kappa-j}^{(n)} w_j \geq (2a_0^{(1)} - a_2^{(3)}) w_1^2 + (2a_1^{(2)} - a_1^{(3)}) w_1 w_2 + (2a_0^{(2)} - a_2^{(3)} - \frac{(a_1^{(3)})^2}{2a_2^{(3)}}) w_2^2$$

$$= (w_1, w_2) \begin{pmatrix} 2a_0^{(1)} - a_2^{(3)} & a_1^{(2)} - \frac{(a_1^{(3)})^2}{2a_2^{(3)}} \\ a_1^{(2)} - a_1^{(3)} & 2a_0^{(2)} - a_2^{(3)} - \frac{(a_1^{(3)})^2}{4a_2^{(3)}} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \geq 0,$$

since the dominant principal minors of the above $2 \times 2$ matrix are greater than zero if $1 < r_k \leq r_{\max} = 1.716$. The proof is completed. \qed

**Remark 2.1.** The generating function of BDF3 kernels $b_{n-k}^{(n)}$ in (1.2) is

$$(2.5) \quad g(x) = a_0^{(n)} + a_1^{(n)} \cos \varphi + a_2^{(n)} \cos (2\varphi) = 2a_2^{(n)} x^2 + a_1^{(n)} x + \left( a_0^{(n)} - a_2^{(n)} \right), \quad n \geq 3$$

with $\cos \varphi = x, x \in [-1, 1], \varphi \in [-\pi, \pi]$. From $2a_2^{(n)} > 0$ and (2.4), it implies that $g(\varphi) > 0$ if $1 < r_k \leq 1.731$. Then BDF3 kernels $b_{n-k}^{(n)}$ in (1.2) are positive definite by Lemma 2.1. In fact, combining with the proof process of Case I in Lemma 2.4, the BDF3 kernels $b_{n-k}^{(n)}$ in (1.2) are positive definite if $r_k \leq 1.731 < \sqrt{3}$. 

2.2. Ratio estimate by Sylvester criterion. From subsection 2.1, we know that the matrix $A$ in (2.2) is positive semi-definite with $r_s \leq 1.716$. Moreover, the BDF3 kernels $b_{n-k}^{(m)}$ in (1.2) are positive definite if $r_k \leq 1.731 < \sqrt{3}$ in (2.5). In fact, we can check that the generating function $g(x) < 0$ in (2.5) if $x = 0.434$, $r_k = 1.732$. However, the positive definiteness with $r_k = 1.732$ in (1.2) by Grenander-Szego theorem is still in doubt. Therefore, we need to look for the upper bound estimate of other forms.

Let $A$ be given in (2.2). From Lemma 2.3, the dominant principal minors of $A + A^T$ are

$$
\det (A + A^T)_{k \times k} = \det L_{k \times k}.
$$

Here the coefficients of $L_{k \times k}$ are

$$
p_1 = 2a_0^{(1)}, \quad q_2 = a_1^{(2)}, \quad p_2 = 2a_0^{(2)} - \frac{1}{p_1}q_2^2,
$$

$$
(2.6)
q_j = a_1^{(j)} - \frac{q_{j-1}}{p_{j-2}}a_2^{(j-1)} \quad \text{and} \quad p_j = 2a_0^{(j)} - \frac{1}{p_{j-2}}(a_2^{(j)})^2 - \frac{1}{p_{j-1}}q_j^2, \quad j \geq 3.
$$

As a counterexample, we take $r_s := r_n = r_{n-1} < \sqrt{3}$ in (2.6). According to Sylvester criterion in Lemma 2.2 and (2.6), we know that there exists a dominant principal minors of $A + A^T$ is negative, since there exists $p_j < 0$, see Figure 2.1. Hence, the matrix $A$ or $B$ in (2.2) is not positive definite if $r_s = 1.732 < \sqrt{3}$. 

![Figure 2.1. The graphs of $p_j$ in (2.6), left and right, respectively, for $r_s \equiv 1.732$ and $r_s \equiv 1.750.\)
From Lemma 2.3, the dominant principal minors of $\tilde{B} + \tilde{B}^T$ are
\[
\det \left( \tilde{B} + \tilde{B}^T \right)_{j \times j} = \det L_{j \times j}.
\]
Here the coefficients of $L$ are computed by
\[
\begin{align*}
p_1 &= \hat{b}_0^{(1)}, \\
p_2 &= \hat{b}_0^{(2)} - \frac{1}{p_1}q_2^2, \\
q_j &= \frac{b_j^{(1)}}{p_j-2} - \frac{q_j-1}{p_j-2}b_1^{(2)} \\
p_j &= \frac{b_j^{(1)}}{p_j-2} - \frac{1}{p_j-2}b_j^{(2)} - \frac{1}{p_j-1}q_j^2, j \geq 3
\end{align*}
\]
with
\[
\begin{align*}
\hat{b}_0^{(1)} &= 1.99/\tau_1, \\
\hat{b}_0^{(2)} &= \frac{1.99 + 3.99r_2}{\tau_2(1 + r_2)}, \\
b_1^{(2)} &= \frac{-r_2^2}{\tau_2(1 + r_2)}, \\
n_0 &= \frac{(1 + r_{n-1})[1.99 + 3.99r_n + r_{n-1}(1.99 + 7.98r_n + 5.99r^2_n)]}{\tau_n(1 + n_{n-1})(1 + r_{n-1})(1 + x_{n-1} + r_{n}r_{n-1})}, \\
b_1^{(n)} &= -\frac{r_n^2((1 + 2r_{n-1} + r_nr_{n-1})^2 - r_{n-1}(1 + r_{n-1}))}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_nr_{n-1})}, \\
b_2^{(n)} &= \frac{r_n^2r_{n-1}^2(1 + r_n^2)}{\tau_n(1 + r_n)(1 + n_{n-1})(1 + r_{n-1} + r_nr_{n-1})} \forall n \geq 3.
\end{align*}
\]
The main result of this part is to estimate the following inequality
\[
\frac{\lambda_{\min}}{\tau_j} \leq p_j \leq \frac{\lambda_{\max}}{\tau_j}, j \geq 1 \text{ with } \lambda_{\min} = 1.99, \lambda_{\max} = 3.99,
\]
it implies that the matrix $A$ or $B$ in (2.2) is positive definite by Sylvester criterion.

3.1. A few technical lemmas. First, we give some lemmas that will be used later.

\textbf{Lemma 3.1.} Let $\Psi(x, y)$ with $(x, y) \in [0, r_s] \times [0, r_s]$, $r_s = 1.405$ be defined by
\[
\Psi(x, y) = \frac{(1 + 2y + xy)^2 - y(1 + y)^2}{(1 + y)(1 + y + xy)} - \frac{\kappa y^4(1 + x)^2}{(1 + y)^2(1 + y + xy)}.
\]
Here the coefficients are defined by
\[
\kappa \in [\kappa_{\min}, \kappa_{\max}], \quad \kappa_{\min} = 0.25, \kappa_{\max} = 1.4.
\]
Then we have
\[
1 \leq \Psi(x, y) \leq 2.7.
\]

\textbf{Proof.} We can check that
\[
\Psi(x, y) = 1 + \frac{(y^2 + y^3 - \kappa y^4)(1 + x)^2 + (1 + x)y(1 + y)^2}{(1 + y)^2(1 + y + xy)} \]
\[
= 1 + \frac{(y^2 + \frac{3}{2}y^3 - \kappa y^4)(1 + x)^2 + (1 + x)y(1 + y)^2 - \frac{1}{2}y^3(1 + x)^2}{(1 + y)^2(1 + y + xy)}
\]
\[
= 1 + \frac{(y^2 + \frac{3}{2}y^3 - \kappa y^4)(1 + x)^2 + \frac{1}{2}(1 - x^2)y^3 + (2 + 2x)y^2 + (1 + x)y}{(1 + y)^2(1 + y + xy)} \geq 1.
\]
Here we use
\[
y^2 + \frac{3}{2}y^3 - \kappa y^4 = y^2 \left(1 + \frac{3}{2}y - \kappa y^2\right) \geq y^2 \left(1 - \frac{3}{2}y(y - 1)\right) \geq 0,
\]
\[
y^2 + \frac{3}{2}y^3 - \kappa y^4 = y^2 \left(1 + \frac{3}{2}y - \kappa y^2\right) \geq y^2 \left(1 - \frac{3}{2}y(y - 1)\right) \geq 0,
\]
and
\[
\frac{1}{2}(1 - x^2) y^3 + (2 + 2x) y^2 + (1 + x) y
= (1 + x) y \left( \frac{1}{2}(1 - x) y^2 + 2 y + 1 \right) \geq (1 + x) y \left(-0.3y^2 + 2y + 1\right) \geq 0.
\]
Similarly, we have
\[
\Psi(x, y) = 2.7 + \frac{(y^3 - y^2 - \kappa y^4)(1 + x)^2 + \Psi_1(x, y)}{(1 + y)^2(1 + y + xy)},
\]
where the quadratic function \(\Psi_1(x, y)\) is
\[
\Psi_1(x, y) = -1.7(1 + y)^3 + y(1 + y)^2 - 0.7xy(1 + y)^2 + 2y^2(1 + x)^2
\leq -1.7(1 + y)^2(y/1.405 + y) + y(1 + y)^2 - 0.7xy(1 + y)^2 + 4.81y^2(1 + x)
\leq -2.909y(1 + y)^2 + y(1 + y)^2 - 0.7xy(1 + y)^2 + 4.81y^2(1 + x)
= y\Psi_2(x, y)
\]
with
\[
\Psi_2(x, y) = -(1.909 + 0.7x)y^2 + (0.992 + 3.41x)y - 1.909 - 0.7x.
\]
Since the discriminant of root formulas of \(\Psi_2(x, y)\) is
\[
\Delta = (0.992 + 3.41x)^2 - 4(1.909 + 0.7x)(1.909 + 0.7x) < 0,
\]
which implies \(\Psi_1(x, y) \leq 0\). Moreover, we have
\[
y^3 - y^2 - \kappa y^4 = y^2(-\kappa y^2 + y - 1) \leq y^2(-0.25y^2 + y - 1) \leq 0.
\]
The proof is completed. \(\Box\)

**Lemma 3.2.** Let \(\psi(x, y)\) with \((x, y) \in [0, r_s] \times [0, r_s], r_s = 1.405\) be defined by
\[
\psi(x, y) = -\frac{x^2[(1 + 2y + xy)^2 - y(1 + y)]}{(1 + x)(1 + y)(1 + y + xy)} + \frac{\kappa_{\max} x^2 y^4(1 + x)}{(1 + y)^2(1 + y + xy)} \text{ with } \kappa_{\max} = 1.4.
\]
Then we have \(\psi(x, y) \leq 0\).

**Proof.** We can check
\[
\psi(x, y) = \frac{x^2}{(1 + x)(1 + y)^2(1 + y + xy)} \psi_1(x, y)
\]
with
\[
\psi_1(x, y) = -(1 + y)^3 - 2y(1 + x)(1 + y)^2 - y^2(1 + x)^2(1 + y) + y(1 + y)^2 + 1.4y^4(1 + x)^2.
\]
Using the above equation and \(1.4y - 2 < 0\), it yields
\[
\psi_1(x, y) \leq -2y(1 + x)(1 + y)^2 - y^2(1 + x)^2(1 + y) + y(1 + y)^2 + 1.4y^3(1 + y)(1 + x)^2
= y(1 + y) \left[-2(1 + x)(1 + y) + y(1 + x)^2 + (1 + y) + (1.4y - 2)y(1 + x)^2\right]
\leq y(1 + y)\psi_2(x, y)
\]
with
\[
\psi_2(x, y) = -2(1 + x)(1 + y) + y(1 + x)^2 + (1 + y).
\]
Since the first derivative of \(\psi_2(x, y)\) with respect to \(y\) is greater than zero. Then we have \(\psi_2(x, y) \leq \psi_2(x, r_s) < 0\). The proof is completed. \(\Box\)
Lemma 3.3. Let $\Phi(x, y)$ with $(x, y) \in [0, r_s] \times [0, r_s]$, $r_s = 1.405$ be defined by

$$\Phi(x, y) = \left[1.99 + 3.99x + y \left(1.99 + 7.98x + 5.99x^2\right)\right] (1 + x)(1 + y)^4(1 + y + xy)$$

$$- \lambda_{\text{min}}(1 + x)^2(1 + y)^4(1 + y + xy)^2 - \frac{1}{\lambda_{\text{min}}} x^3 y^5 (1 + x)^4 (1 + y)^2$$

$$- \frac{1}{\lambda_{\text{min}}} x^3 \left[(1 + 2y + 2xy)(1 + y)^2 + y^2 (1 + x)^2 (1 + y - \kappa_{\text{min}}y^2)\right]^2$$

with $\lambda_{\text{min}} = 1.99$, $\kappa_{\text{min}} = 0.25$. Then we have $\Phi(x, y) \geq 0$.

Proof. According to

$$1 \leq 1 + y - \kappa_{\text{min}}y^2 \leq 1 + r_s - \kappa_{\text{min}}r_s^2 < 1.912,$$

and

$$1.99 + 3.99x + y \left(1.99 + 7.98x + 5.99x^2\right) - \lambda_{\text{min}}(1 + x)(1 + y + xy) = 2x(1 + 2y + 2xy),$$

it leads to

$$\lambda_{\text{min}} \Phi(x, y) \geq 3.98x(1 + 2y + 2xy)(1 + x)(1 + y)^4(1 + y + xy) - x^3 y^5 (1 + x)^4 (1 + y)^2$$

$$- x^3 \left[(1 + 2y + 2xy)(1 + y)^2 + 1.912y^2 (1 + x)^2\right]^2$$

$$= x(1 + y)^4 \Phi_1(x, y) + xy(1 + x)(1 + y)^2 \Phi_2(x, y) + xy^2(1 + x)^2 \Phi_3(x, y).$$

Here

$$\Phi_1(x, y) = -1.13x^2 y(1 + x) - x^2 + 3.98x + 3.98;$$

$$\Phi_2(x, y) = 11.94(1 + x)(1 + y)^2 - 2.87x^2(1 + y)^2$$

$$- 2.793x^2 y(1 + x)(1 + y)^2 - 2.824x^2 y(1 + x);$$

$$\Phi_3(x, y) = 7.96(1 + x)(1 + y)^4 - 1.207x^2(1 + y)^4 - x^2 y^3 (1 + x)^2 (1 + y)^2$$

$$- 7.648x^2 y(1 + x)(1 + y)^2 - 2.655744x^2 y(1 + x)^2.$$

We can check $\Phi_1(x, y) \geq -1.13x^2 r_s (1 + r_s) - x^2 + 3.98x + 3.98 > 0$ and

$$\Phi_2(x, y) \geq 11.94(1 + x)(1 + y)^2 - 2.87x^2(1 + y)^2 - 6.718x^2 y(1 + y)^2 - 9.197x^2 y$$

$$= x(1 + y)^2 (11.94 - 6.048xy) + h(x, y) \geq h(x, y)$$

with $h(x, y) = 11.94(1 + y)^2 - 2.87x^2(1 + y)^2 - 0.67x^2 y(1 + y)^2 - 9.197x^2 y$. Since the first derivative of $h(x, y)$ with respect to $x$ is less than zero. It implies that $h(x, y) \geq h(r_s, y)$. Moreover, the first derivative of $h(r_s, y)$ with respect to $y$ is also less than zero. Then

$$\Phi_2(x, y) \geq h(x, y) \geq h(r_s, y) \geq h(r_s, r_s) > 0.$$

On the other hand, there exists

$$\Phi_3(x, y) \geq xy g(x, y)$$

with

$$g(x, y) = 7.96 \left(\frac{1}{r_s} + 1\right) (1 + y)^4 - 1.207x(1 + y)^4 - xy^3 (1 + r_s)^2 (1 + y)^2$$

$$- 7.648xy(1 + r_s)(1 + y)^2 - 3.655744xy^2 (1 + r_s)^2.$$
Since the first derivative of \( g(x, y) \) with respect to \( x \) is less than zero. It implies that \( g(x, y) \geq g(r_s, y) \). Furthermore, we have \( g(r_s, y) \geq g(r_s, r_s) > 0 \). Hence, there exists
\[
\Phi_3(x, y) \geq xg(x, y) \geq xg(r_s, y) \geq xg(r_s, r_s) \geq 0.
\]
The proof is completed.

□

**Lemma 3.4.** Let \( \phi(x, y) \) with \( (x, y) \in [0, r_s] \times [0, r_s] \), \( r_s = 1.405 \) be defined by
\[
\phi(x, y) = \left[ 1.99 + 3.99x + y \left( 1.99 + 7.98x + 5.99x^2 \right) \right] (1 + x)(1 + y)^4(1 + y + xy)
\]
\[
- \lambda_{\text{max}}(1 + x)^2(1 + y)^4(1 + y + xy)^2 - \frac{1}{\lambda_{\text{max}}} x^3 y^5(1 + x)^4(1 + y)^2
\]
\[
- \frac{1}{\lambda_{\text{max}}} x^3 \left[ (1 + 2y + 2xy)(1 + y)^2 + y^2 (1 + x)^2 (1 + y - \kappa_{\text{max}}y^2) \right]^2
\]
with \( \lambda_{\text{max}} = 3.99, \kappa_{\text{max}} = 1.4 \). Then we have \( \phi(x, y) \leq 0 \).

**Proof.** Using
\[
\left[ (2y + 2xy)(1 + y)^2 + y^2 (1 + x)^2 (1 + y - \kappa_{\text{max}}y^2) \right] - 2y^2(1 + x)(1 + y)
\]
\[
\geq y(1 + x) \left[ 2(1 + y)^2 + y (1 + y - \kappa_{\text{max}}y^2) - 2y(1 + y) \right] \geq 0,
\]
and
\[
1.99 + 3.99x + y \left( 1.99 + 7.98x + 5.99x^2 \right) - \lambda_{\text{max}}(1 + x)(1 + y + xy) = -2 - 2y + 2x^2 y,
\]
it yields
\[
\lambda_{\text{max}} \phi(x, y) \leq \lambda_{\text{max}} \left( -2 - 2y + 2x^2 y \right)(1 + x)(1 + y)^4(1 + y + xy) - 4x^3 y^4 (1 + x)^2 (1 + y)^2
\]
\[
= (1 + x)^2(1 + y)^2 y \phi_1(x, y) + (1 + x)(1 + y)^4 \phi_2(x, y).
\]
Here the functions \( \phi_1(x, y) \) and \( \phi_2(x, y) \) are, respectively, defined by
\[
\phi_1(x, y) = 7.98x^2 y(1 + y)^2 - 7(1 + y)^3 - 4x^3 y^3,
\]
and
\[
\phi_2(x, y) = 7.98x^2 y - 7.98(1 + y) - 0.98y(1 + y)(1 + x) \leq \phi_3(x, y)
\]
with
\[
\phi_3(x, y) = 7.98x^2 y - 7.98(1 + y) - 0.98y(1 + y).
\]
Since the first derivative of \( \phi_1(x, y) \) and \( \phi_3(x, y) \) with respect to \( x \) is greater than zero. Hence
\[
\phi_1(x, y) \leq \phi_1(r_s, y) \leq \phi_1(r_s, r_s) \leq 0,
\]
\[
\phi_3(x, y) \leq \phi_3(r_s, y) \leq \phi_3(r_s, r_s) \leq 0.
\]
The proof is completed. □
3.2. Estimate for variable time-step ratio by Sylvester criterion. We next prove the matrix $A$ or $B$ in (2.2) is positive definite by Sylvester criterion.

**Lemma 3.5.** For any adjacent time-step ratios $0 < r_k \leq r_s = 1.405$, $k \geq 2$, there exists

\[(3.4) \quad b_1^{(j)} + \mu_j \leq q_j \leq b_1^{(j)} + \nu_j \leq 0, \quad j \geq 3\]

with

\[(3.5) \quad \mu_j = \frac{\kappa_{\min} r_j^2 r_{j-1}^4 (1 + r_j)}{\tau_j (1 + r_{j-1})^2 (1 + r_j - r_j r_{j-1})}, \quad \nu_j = \frac{\kappa_{\max} r_j^2 r_{j-1}^4 (1 + r_j)}{\tau_j (1 + r_{j-1})^2 (1 + r_j - r_j r_{j-1})},\]

and

\[(3.6) \quad \frac{\lambda_{\min}}{\tau_j} \leq p_j \leq \frac{\lambda_{\max}}{\tau_j}, \quad j \geq 1.\]

Here the coefficients are defined by

\[\kappa_{\min} = 0.25, \quad \kappa_{\max} = 1.4 \quad \text{and} \quad \lambda_{\min} = 1.99, \quad \lambda_{\max} = 3.99.\]

**Proof.** From (3.2) and (3.3), we obtain $p_1 = \frac{1.99}{\tau_1}$, $q_2 = \frac{-r_2^2}{\tau_2 (1 + r_2)}$ and

\[\frac{\lambda_{\max}}{\tau_2} \geq \frac{\lambda_{\max}}{\tau_2} - \frac{2 + 2r_2 + \frac{1}{1.99} r_2^3}{\tau_2 (1 + r_2)^2} = p_2 = \frac{\lambda_{\min}}{\tau_2} + \frac{2r_2 + 2r_2^2 - \frac{1}{1.99} r_2^3}{\tau_2 (1 + r_2)^2} \geq \frac{\lambda_{\min}}{\tau_2}.\]

Next we prove (3.4) and (3.6) by mathematical induction.

For $j = 3$, using Lemma 3.2, we have

\[(3.7) \quad b_1^{(3)} + \mu_3 \leq b_1^{(3)} + \frac{1}{1.99} r_2^4 r_3^2 (1 + r_3)}{\tau_3 (1 + r_2)^2 (1 + r_2 + r_2 r_3)} = q_3 \leq b_1^{(3)} + \nu_3 = \psi(r_3, r_2) \leq 0.\]

According to (3.2), (3.3) and (3.7), it yields

\[
p_3 \geq \frac{\tau_1}{\lambda_{\min}} \left( b_1^{(3)} \right)^2 - \frac{\tau_2}{\lambda_{\min}} \left( b_1^{(3)} + \mu_3 \right)^2 = \frac{\tau_1}{\lambda_{\min}} \left( b_1^{(3)} \right)^2 - \frac{\tau_2}{\lambda_{\min}} \left( b_1^{(3)} + \mu_3 \right)^2 + \frac{1}{\tau_3 (1 + r_3)^2 (1 + r_2)^4 (1 + r_2 + r_2 r_3)^2} \cdot \Phi(r_3, r_2) \geq \frac{\lambda_{\min}}{\tau_3},\]

with $\Phi(r_3, r_2) \geq 0$ in Lemma 3.3.

On the other hand, using (3.2), (3.3) and (3.7), one has

\[
p_3 \leq \frac{\tau_1}{\lambda_{\max}} \left( b_1^{(3)} \right)^2 - \frac{\tau_2}{\lambda_{\max}} \left( b_1^{(3)} + \nu_3 \right)^2 \leq \frac{\tau_1}{\lambda_{\max}} \left( b_1^{(3)} \right)^2 - \frac{\tau_2}{\lambda_{\max}} \left( b_1^{(3)} + \nu_3 \right)^2 + \frac{1}{\tau_3 (1 + r_3)^2 (1 + r_2)^4 (1 + r_2 + r_2 r_3)^2} \cdot \phi(r_3, r_2) \leq \frac{\lambda_{\max}}{\tau_3},\]

with $\phi(r_3, r_2) \leq 0$ in Lemma 3.4.

Supposing that (3.4) and (3.6) hold for $j = 4, \ldots, n - 1$, namely,

\[(3.8) \quad b_1^{(j)} + \mu_j \leq q_j \leq b_1^{(j)} + \nu_j \leq 0 \quad \text{and} \quad \frac{\lambda_{\min}}{\tau_j} \leq p_j \leq \frac{\lambda_{\max}}{\tau_j}, \quad 4 \leq j \leq n - 1.\]
According to (3.2), (3.3), (3.8) and Lemma 3.2, there exists
\[ q_n = b_1^{(n)} - \frac{q_{n-1}}{p_{n-2}} b_2^{(n)} \leq b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\text{min}}} (-q_{n-1}) b_2^{(n)} \leq b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\text{min}}} (-b_1^{(n-1)} - \nu_{n-1}) b_2^{(n)} \]
\[ = b_1^{(n)} + \frac{\Psi(r_{n-1}, r_{n-2})}{\lambda_{\text{min}}} \frac{r_n^2 r_{n-1}^4 (1 + r_n)}{\tau_n (1 + r_{n-1})^2 (1 + r_{n-1} + r_n r_{n-1})} \leq b_1^{(n)} + \nu_n = \psi(r_n, r_{n-1}) \leq 0, \]
where \( \Psi(r_{n-1}, r_{n-2}) \) and \( \nu_n \) are, respectively, defined by Lemma 3.1 and (3.5).

On the other hand, using (3.2), (3.3) and (3.8), we have
\[ q_n = b_1^{(n)} - \frac{q_{n-1}}{p_{n-2}} b_2^{(n)} \geq b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\text{max}}} (-q_{n-1}) b_2^{(n)} \geq b_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\text{max}}} (-b_1^{(n-1)} - \nu_{n-1}) b_2^{(n)} \]
\[ = b_1^{(n)} + \frac{\Psi(r_{n-1}, r_{n-2})}{\lambda_{\text{max}}} \frac{r_n^2 r_{n-1}^4 (1 + r_n)}{\tau_n (1 + r_{n-1})^2 (1 + r_{n-1} + r_n r_{n-1})} \geq b_1^{(n)} + \mu_n, \]
where \( \Psi(r_{n-1}, r_{n-2}) \) and \( \mu_n \) are, respectively, defined by Lemma 3.1 and (3.5).

From (3.2), (3.3) and (3.8), it yields
\[ p_n = \hat{b}_0^{(n)} - \frac{1}{p_{n-2}} (b_2^{(n)})^2 - \frac{1}{p_{n-1}} q_n^2 \geq b_0^{(n)} - \frac{\tau_{n-2}}{\lambda_{\text{min}}} (b_2^{(n)})^2 - \frac{\tau_{n-1}}{\lambda_{\text{min}}} (b_1^{(n)} + \mu_n)^2 \]
\[ = \frac{\lambda_{\text{min}}}{\tau_n} + \frac{1}{\tau_n (1 + r_n)^2 (1 + r_{n-1})^4 (1 + r_{n-1} + r_n r_{n-1})^2} \cdot \Phi(r_n, r_{n-1}) \geq \frac{\lambda_{\text{min}}}{\tau_n} \]
with \( \Phi(r_n, r_{n-1}) \geq 0 \) in Lemma 3.3. Similarly, we have
\[ p_n = \hat{b}_0^{(n)} - \frac{1}{p_{n-2}} (b_2^{(n)})^2 - \frac{1}{p_{n-1}} q_n^2 \leq b_0^{(n)} - \frac{\tau_{n-2}}{\lambda_{\text{max}}} (b_2^{(n)})^2 - \frac{\tau_{n-1}}{\lambda_{\text{max}}} (b_1^{(n)} + \nu_n)^2 \]
\[ = \frac{\lambda_{\text{max}}}{\tau_n} + \frac{1}{\tau_n (1 + r_n)^2 (1 + r_{n-1})^4 (1 + r_{n-1} + r_n r_{n-1})^2} \cdot \phi(r_n, r_{n-1}) \leq \frac{\lambda_{\text{max}}}{\tau_n} \]
with \( \phi(r_n, r_{n-1}) \leq 0 \) in Lemma 3.4. The proof is completed.
□

**Remark 3.1.** In fact, the upper ratio \( r_s = 1.405 \) is the root of the polynomial function \( \Phi(x, x) \) arising from Lemma 3.3.

### 4. Estimate for variable adjacent time-step ratio of WSBDF3

As is well known, the stability of the 3-step backward differentiation formula (BDF3) on variable grids for a parabolic problem is analyzed in [4] under the condition \( r_k < 1.199 \). In Section 3, we prove that the BDF3 scheme is unconditionally stable under the time-step ratio \( r_k \leq 1.405 \) by Sylvester criterion. Moreover, the upper bound of the ratio \( r_k \) is less than \( \sqrt{3} \) for BDF3. In this section, we introduce a weighted and shifted BDF3 scheme, which is unconditionally stable under the time-step ratio \( r_k \leq 1.771 \) by Sylvester criterion.

#### 4.1. Weighted and shifted BDF3 scheme.

From (1.2), we know that the BDF3 scheme at \( t_n \) is defined by
\[ D_3 v^n = (\Pi_{n,3} v') (t_n) = b_0^{(n)} \nabla_\tau v^n + b_1^{(n)} \nabla_\tau v^{n-1} + b_2^{(n)} \nabla_\tau v^{n-2} = \sum_{k=1}^n b_{n-k}^{(n)} \nabla_\tau v^k, \quad n \geq 3. \]
Based on the idea of [6], we construct the following shifted BDF3 formula at \( t_{n-1} \), namely,

\[
\tilde{D}_3v^n = (\Pi_{n,3}v)'(t_{n-1}) = \tilde{b}_0^{(n)} \nabla_{\tau} v^n + \tilde{b}_1^{(n)} \nabla_{\tau} v^{n-1} + \tilde{b}_2^{(n)} \nabla_{\tau} v^{n-2} = \sum_{k=1}^{n} \tilde{b}_{n-k}^{(n)} \nabla_{\tau} v^k, \quad n \geq 3.
\]

Here the coefficients are computed by

\[
\begin{align*}
\tilde{b}_0^{(n)} &= \frac{(1 + r_{n-1})^2}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\
\tilde{b}_1^{(n)} &= \frac{r_n^2 [1 + 3r_{n-1}(1 + r_{n-1}) + r_n r_{n-1}(1 + 2r_{n-1})]}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\
\tilde{b}_2^{(n)} &= -\frac{r_n^2 r_{n-1}^2 (1 + r_n)}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})} \quad \text{with} \quad \tilde{b}_j^{(n)} = 0, \quad j \geq 3.
\end{align*}
\]

Then the weighted and shifted BDF3 (WSBDF3) operator is defined by

\[
D_3v^n := \theta D_3v^n + (1 - \theta) \tilde{D}_3v^n \quad \text{with} \quad \theta \in [1/2, 1], \quad n \geq 3.
\]

Namely,

\[
(4.1) \quad D_3v^n = w_0^{(n)} \nabla_{\tau} v^n + w_1^{(n)} \nabla_{\tau} v^{n-1} + w_2^{(n)} \nabla_{\tau} v^{n-2} = \sum_{k=1}^{n} w_{n-k}^{(n)} \nabla_{\tau} v^k, \quad n \geq 3
\]

with the coefficients

\[
(4.2) \quad w_0^{(n)} = \frac{(1 + r_{n-1}) [1 + 2\theta r_n + r_{n-1}(1 + 4\theta r_n + 3\theta r_n^2)]}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\
\quad w_1^{(n)} = -\frac{r_n^2 [2\theta - 1 + 3(2\theta - 1)r_{n-1}(1 + r_{n-1}) + (3\theta - 1)r_n r_{n-1}(1 + 2r_{n-1}) + \theta r_n^2]}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})}, \\
\quad w_2^{(n)} = \frac{r_n^2 r_{n-1}^2 (1 + r_n)(2\theta - 1 + \theta r_n)}{\tau_n(1 + r_n)(1 + r_{n-1})(1 + r_{n-1} + r_n r_{n-1})} \quad \text{with} \quad w_j^{(n)} = 0, \quad j \geq 3.
\]

Since WSBDF3 method needs three starting values, for concreteness, we use WSBDF1 scheme and WSBDF2 scheme [6], respectively, to compute the first-level solution \( u^1 \) and second-level solution \( u^2 \), namely,

\[
(4.3) \quad D_3v^1 = \nabla_{\tau} v^1/\tau, \quad D_3v^2 = 1 + \frac{2\theta r_2}{\tau_2(1 + r_2)} \nabla_{\tau} v^2 + \frac{(1 - 2\theta) r_2^2}{\tau_2(1 + r_2)} \nabla_{\tau} v^1, \quad \theta \in [1/2, 1].
\]

Then we recursively define a sequence of approximations \( u^n \) to the nodal values \( a(t^n) \) of the exact solution by WSBDF3 method

\[
(4.4) \quad D_3u^n + \theta Au^n + (1 - \theta) Au^{n-1} = \theta f^n + (1 - \theta) f^{n-1}, \quad n \geq 1
\]

with the initial data \( u^0 = u_0 \) and the exterior force \( f^n = f(t_n) \). In particular, WSBDF3 scheme (4.4) reduces to the BDF3 method (1.5) if \( \theta = 1 \).

**Remark 4.1.** Let \( \tau \) be the uniform time stepsize and the initial value problem of (1.1) be the form \( u'(t) = f(u, t) \). Then (4.4) reduces to the following simple form

\[
(4.5) \quad \left( \begin{array}{c} 
\frac{3}{2} \theta + \frac{1}{3} \end{array} \right) u_{n+3} + \left( -\frac{7}{2} \theta + \frac{1}{2} \right) u_{n+2} + \left( \frac{5}{2} \theta - 1 \right) u_{n+1} + \left( -\frac{1}{2} \theta + \frac{1}{6} \right) u_n = \tau (\theta f_{n+3} + (1 - \theta) f_{n+2})
\]


with the characteristic polynomials
\[
\rho(\xi) = \left(\frac{3}{2} \theta + \frac{1}{3}\right) \xi^3 + \left(-\frac{7}{2} \theta + \frac{1}{2}\right) \xi^2 + \left(\frac{5}{2} \theta - 1\right) \xi + \left(-\frac{1}{2} \theta + \frac{1}{6}\right),
\]
\[
\sigma(\xi) = \theta \xi^3 + (1 - \theta) \xi^2.
\]
In fact, the above scheme (4.5) has been discussed in [15]. Moreover, the coefficients of WSBDF3 operator (4.1) share similarities with the implicit-explicit multistep methods in [20], where the zero-stability is studied for ODEs; and its stability analysis remains an open question for PDEs.

From Theorem 2.2 in [9] and Theorem 1 in [15], we know that the linear method is \(A(\alpha)\)-stable, which requires the roots of the second characteristic polynomial \(\sigma(\xi)\) lie on or within the unit circle. Namely,
\[
\xi = \left|\frac{1 - \theta}{\theta}\right| \leq 1 \text{ if and only if } \theta \geq \frac{1}{2}.
\]
Similar discussion is given in Remark 2.1 by Grenander-Szegö theorem, we find the adjacent time-step ratio \(r_k := \tau_k/\tau_{k-1}\) is increasing when \(\theta\) decreases to \(\frac{1}{2}\) for WSBDF3 scheme (4.4), see Figure 4.1.

![Figure 4.1](image-url)

**Figure 4.1.** WSBDF3: Ratio \(r_k := \tau_k/\tau_{k-1}\) is increasing if \(\theta\) decreases to \(\frac{1}{2}\).

Following the approach of [6, 16], the DOC kernels \(\{\theta_{n-k}^{(n)}\}_{k=1}^{n}\) for \(1 \leq k \leq n - 1\) are defined by

\[
\theta_0^{(n)} := -\frac{1}{w_0^{(n)}} \text{ and } \theta_{n-k}^{(n)} := -\frac{1}{w_0^{(k)}} \sum_{j=k+1}^{n} \theta_{n-j}^{(n)} w_{j-k}^{(j)} = -\frac{\theta_{n-k-1}^{(n)} w_{1}^{(k+1)} + \theta_{n-k-2}^{(n)} w_{2}^{(k+2)}}{w_0^{(k)}}.
\]
Moreover, the DOC kernels \( \{\theta^{(n)}_{n-k}\}_{k=1}^{n} \) satisfy the discrete orthogonal identity

\[
\sum_{j=k}^{n} \theta^{(n)}_{n-j} w^{(n)}_{j-k} \equiv \delta_{nk} \text{ for } 1 \leq k \leq n.
\]

For convenience, we introduce the following matrices:

\[
W := \begin{pmatrix}
w^{(1)}_0 & w^{(2)}_0 & w^{(3)}_0 \\
\vdots & \ddots & \vdots \\
w^{(n)}_0 & w^{(n)}_1 & w^{(n)}_n
\end{pmatrix}
\quad \text{and} \quad
\Theta := \begin{pmatrix}
\theta^{(1)}_0 & \theta^{(2)}_0 & \theta^{(3)}_0 \\
\vdots & \ddots & \vdots \\
\theta^{(n)}_{n-1} & \theta^{(n)}_{n-2} & \theta^{(n)}_n
\end{pmatrix},
\]

where the discrete convolution kernels \( w^{(n)}_k \) and the DOC kernels \( \{\theta^{(n)}_{n-k}\}_{k=1}^{n} \) are defined in (4.2) and (4.6), respectively. It follows from the discrete orthogonal identity (4.7) that

\[
\Theta = W^{-1}.
\]

4.2. Estimate for variable time-step ratio by Sylvester criterion. In this section, we focus on the optimal case \( \theta = \frac{1}{2} \) in (4.4) by Remark 4.1. More general \( \theta \) can be similarly studied. Let \( W \) and \( \Lambda \) be given in (4.8) and (2.1), respectively. Let the matrix be

\[
\tilde{W} = W - \epsilon \Lambda^{-1} \text{ with } \epsilon = 1/200.
\]

From Lemma 2.3, the dominant principal minors of \( \tilde{W} + \tilde{W}^T \) are

\[
\det (\tilde{W} + \tilde{W}^T)_{j \times j} = \det L_{j \times j}.
\]

Here the elements of \( L \) are computed by

\[
p_1 = \tilde{w}^{(1)}_0, \quad q_2 = w^{(2)}_1 = 0, \quad p_2 = \tilde{w}^{(2)}_0 - \frac{1}{p_1} q_2, \quad p_j = \tilde{w}^{(j)}_0 - \frac{1}{p_{j-2}} (w^{(j)}_0)^2 - \frac{1}{p_{j-1}} q_j^2, \quad j \geq 3
\]

with

\[
\tilde{w}^{(1)}_0 = 1.99/\tau_1, \quad \tilde{w}^{(2)}_0 = 1.99/\tau_2,
\]

\[
\tilde{w}^{(n)}_0 = \frac{1 + r_{n-1}}{\tau_n (1 + r_n) (1 + r_{n-1})} \left[ 1.99 + 1.99 r_n + r_{n-1} (1.99 + 3.98 r_n + 2.99 r_n^2) \right],
\]

\[
w^{(1)}_0 = -\frac{1/2 r^3 n^{-1}}{\tau_n (1 + r_n) (1 + r_{n-1}) (1 + r_{n-1} + r_n r_{n-1})}, \quad n \geq 3.
\]

Lemma 4.1. Let \( \varphi(x, y) \) with \( (x, y) \in [0, r_s] \times [0, r_s], r_s = 1.771 \) be defined by

\[
\varphi(x, y) = (1 + x)(1 + y)^2(1 + y + xy) - \frac{1}{4\lambda_{\min}} x^3 y^4 (1 + x)^2 - \frac{1}{4\lambda_{\min}} x^3 y (1 + 2y + xy)^2
\]

with \( \lambda_{\min} = 1.99. \) Then we have \( \varphi(x, y) \geq 0. \)
Proof. We can check \( \varphi(x, y) = (1 + y)\varphi_1(x, y) \) with
\[
\varphi_1(x, y) = (1 + x)(1 + y) + y(1 + x)^2(1 + y) - \frac{1}{4\lambda_{\min}}x^3y(1 + y) - \frac{1}{2\lambda_{\min}}x^3y^2(1 + x) - \frac{1}{4\lambda_{\min}}x^3y^3(1 + x)^2
\]
\[
\geq (x/r_s + x)(y/r_s + y) + y(1 + x)(x/r_s + x)(1 + y)
\]
\[
- \frac{1}{4\lambda_{\min}}xyr_s^2(1 + r_s) - \frac{1}{2\lambda_{\min}}xy^2r_s^2(1 + r_s) - \frac{1}{4\lambda_{\min}}x^2y^2r_s^2(1 + r_s)^2 = xy\varphi_2(x, y).
\]
Here the function \( \varphi_2(x, y) \) is computed by
\[
\varphi_2(x, y) = (1/r_s + 1)^2 + (1/r_s + 1)(1 + x)(1 + y)
\]
\[
- \frac{1}{4\lambda_{\min}}r_s^2(1 + r_s) - \frac{1}{2\lambda_{\min}}r_s^2y(1 + r_s) - \frac{1}{4\lambda_{\min}}r_s^2xy(1 + r_s)^2.
\]
Since the first derivative of \( \varphi_2(x, y) \) with respect to \( y \) is less than zero. Then we have \( \varphi_2(x, y) \geq \varphi_2(x, r_s) \geq \varphi_2(r_s, r_s) \geq 0 \).

The proof is completed.

\[\square\]

Lemma 4.2. Let \( \ell(x, y) \) with \( (x, y) \in [0, r_s] \times [0, r_s] \), \( r_s = 1.771 \) be defined by
\[
\ell(x, y) = x^2y(1 + 2y + xy) - \frac{\lambda_{\min}}{2}(1 + x)(1 + y)(1 + y + xy)
\]
with \( \lambda_{\min} = 1.99 \). Then we have \( \ell(x, y) \leq 0 \).

Proof. We can check
\[
\ell(x, y) = xy(1 + y) (0.35x - 0.65) + (1 + x) \left( x^2y^2 - 0.995(1 + y)^2 - 0.345(1 + y)xy \right)
\]
\[
= xy(1 + y) (0.35x - 0.65) + (1 + x) \left[ \ell_1(x, y) + xy\ell_2(x, y) \right]
\]
with \( \ell_1(x, y) = 0.75x^2y^2 - 0.995(1 + y)^2 \) and \( \ell_2(x, y) = 0.25xy - 0.345(1 + y) \).

Since the first derivative of \( \ell_1(x, y) \) and \( \ell_2(x, y) \) with respect to \( x \) are, respectively, greater than zero, which leads to
\[
\ell_1(x, y) \leq \ell_1(r_s, y) \leq 0, \quad \ell_2(x, y) \leq \ell_2(r_s, y) \leq 0.
\]
The proof is completed.

\[\square\]

Lemma 4.3. For any adjacent time-step ratios \( 0 < r_k \leq r_s = 1.771, k \geq 2 \), there exists
\[
w_1^{(j)} \leq q_j \leq 0, \quad j \geq 2 \) and \( p_j \geq \frac{\lambda_{\min}}{r_j}, \quad j \geq 1 \) with \( \lambda_{\min} = 1.99 \).

(4.12)

Proof. From (4.10) and (4.11), there exists \( p_1 = \hat{w}_0^{(1)} = \frac{\lambda_{\min}}{r_1}, q_2 = w_1^{(2)} = 0 \) and \( p_2 = \frac{\lambda_{\min}}{r_2} \).

We next prove the desired result by mathematical induction. For \( j = 3 \), using (4.10) and (4.11), it yields
\[
q_3 = w_1^{(3)} - \frac{q_2}{p_1}w_2^{(3)} = w_1^{(3)} \leq 0.
\]
According to (4.10), (4.11) and the above equation, we have
\[ p_3 = \frac{\hat{w}_0^{(3)}}{p_1} - \frac{1}{p_2} (w_2^{(3)})^2 - \frac{1}{p_3} q_3^2 = \frac{\tau_1}{\lambda_{\min}} (w_2^{(3)})^2 - \frac{\tau_2}{\lambda_{\min}} (w_1^{(3)})^2 \]
\[ = \frac{\lambda_{\min}}{\tau_3} + \frac{r_3^2 r_2}{\tau_3 (1 + r_3)^2 (1 + r_2)^2 (1 + r_2 + r_3 r_2)^2} \varphi (r_3, r_2) \geq \frac{\lambda_{\min}}{\tau_3} \]
with \( \varphi (r_3, r_2) \geq 0 \) in Lemma 4.1.

Supposing that (4.12) hold for \( j = 4, \ldots, n - 1 \), namely,
\[ w_1^{(j)} \leq q_j \leq 0, \text{ and } p_j \geq \frac{\lambda_{\min}}{\tau_j}, \quad 4 \leq j \leq n - 1. \]

From (4.10) and (4.11), there exists
\[ w_1^{(n)} \leq q_n = w_1^{(n)} - \frac{q_{n-1}}{p_{n-2}} w_2^{(n)} \leq w_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\min}} (-q_{n-1}) w_2^{(n)} \]
\[ \leq w_1^{(n)} + \frac{\tau_{n-2}}{\lambda_{\min}} (-w_1^{(n-1)}) w_2^{(n)} \leq w_1^{(n)} + \frac{1}{4} w_2^{(n)} \]
\[ = -1/2 r_3^2 r_{n-1} (1 + r_{n-1}) - 1/8 r_3^2 r_{n-1}^2 (1 + r_n) (4 - r_{n-1}) \]
\[ \tau_n (1 + r_n) (1 + r_{n-1}) (1 + r_{n-1} + r_n r_{n-1}) \]
\[ \leq 0, \]
since
\[ \frac{\tau_{n-2}}{\lambda_{\min}} (-w_1^{(n-1)}) = \frac{1}{4} + \frac{\ell (r_{n-1}, r_{n-2})}{2 \lambda_{\min} (1 + r_{n-1}) (1 + r_{n-2}) (1 + r_{n-2} + r_{n-1} r_{n-2})} \leq \frac{1}{4} \]
with \( \ell (r_{n-1}, r_{n-2}) \leq 0 \) in Lemma 4.2.

On the other hand, from (4.10) and (4.11), we have
\[ p_n = \frac{\hat{w}_0^{(n)}}{p_{n-2}} - \frac{1}{p_{n-1}} (w_2^{(n)})^2 - \frac{1}{p_{n-1}^2} q_n^2 \geq \frac{\tau_{n-2}}{\lambda_{\min}} (w_2^{(n)})^2 - \frac{\tau_{n-1}}{\lambda_{\min}} (w_1^{(n)})^2 \]
\[ = \frac{\lambda_{\min}}{\tau_n} + \frac{r_3^2 r_{n-1}}{\tau_n (1 + r_n)^2 (1 + r_{n-1})^2 (1 + r_{n-1} + r_n r_{n-1})^2} \varphi (r_n, r_{n-1}) \geq \frac{\lambda_{\min}}{\tau_n} \]
with \( \varphi (r_n, r_{n-1}) \geq 0 \) in Lemma 4.1. The proof is completed. \( \square \)

**Remark 4.2.** In fact, the upper ratio \( r_s = 1.771 \) is the root of the polynomial function \( \varphi (x, x) \) arising from Lemma 4.1.

### 5. Stability and Convergence Analysis

Let \( \langle \cdot, \cdot \rangle \) be the usual inner product in the space \( L^2 (\Omega) \)
\[ \langle u, v \rangle = \int_{\Omega} u(x) v(x) dx, \quad \| u \| = (u, u)^{1/2}. \]

Denote \( \langle \cdot, \cdot \rangle \) the classical Euclidean scalar product
\[ \langle \mu, \nu \rangle = \nu^T \mu = \sum_{k=1}^{n} \mu^k \nu^k, \quad |\mu| = \langle \mu, \mu \rangle^{1/2} \]
with \( \mu = (\mu^1, \mu^2, \ldots, \mu^n)^T \) and \( \nu = (\nu^1, \nu^2, \ldots, \nu^n)^T \). From [17, pp. 23-24], we know that the spectral norm of the matrix \( A \in \mathbb{R}^{n \times n} \) satisfies
\[ |A\mu| \leq |A||\mu| \text{ with } |A| = \sqrt{\rho (A^T A)}. \]
Here the spectral radius $\rho(A)$ is denoted by the maximum module of the eigenvalues of $A$.

**Definition 5.1.** Let $A$ and $B$ be two real $n \times n$ matrices. Then, $A > B$ ($\geq B$) if $A - B$ is positive definite (positive semi-definite).

Let $I$ be the $n \times n$ identity matrix and $\Lambda = \text{diag}(\tau_1, \tau_2, \ldots, \tau_n)$ in (2.1). Then we have the following results.

**Lemma 5.1.** Let $W > c\Lambda^{-1}$, $c > 0$. Then $\mathcal{A} := \Lambda^{1/2}W\Lambda^{1/2} > cI$.

**Proof.** Taking $x = \Lambda^{1/2}y$ with $x \neq 0$, it yields
\[
0 < x^T (W - c\Lambda^{-1}) x = y^T \Lambda^{1/2} (W - c\Lambda^{-1}) \Lambda^{1/2} y = y^T (\Lambda^{1/2}W\Lambda^{1/2} - cI) y.
\]
The proof is completed. \hfill \Box

**Lemma 5.2** (Spectral norm inequality). Let $A > cI$, $c > 0$. Then the spectral norm $|A^{-1}| < c^{-1}$.

**Proof.** Since
\[
x^T (A - cI) x > 0, \quad x^T (A^T - cI) x > 0 \quad \forall x \neq 0.
\]
Using the classical Euclidean scalar product, it yields
\[
0 < |(A - cI) x|^2 = x^T (A^T - cI) (A - cI) x = x^T (A^T A - cA^T - cA + c^2 I) x
\]
\[
= x^T (A^T A - c^2 I - cA^T - cA + 2c^2 I) x \quad \forall x \neq 0.
\]
According to the above inequalities, we have
\[
x^T (A^T A - c^2 I) x > c x^T (A^T + A - 2cI) x > 0 \quad \forall x \neq 0,
\]
which implies that the matrix $A^T A$ is symmetric positive definite. Let $\{\mu_i\}_{i=1}^n$ be an orthonormal set of eigenvectors of $A^T A$, i.e., $A^T A\mu_i = \lambda_i \mu_i$ with $0 < \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$. Thus, we obtain
\[
x^T A^T A x = \sum_{i=1}^n c_i^2 \lambda_i, \quad x^T x = \sum_{i=1}^n c_i^2 \quad \forall x = \sum_{i=1}^n c_i \mu_i.
\]
From (5.2) and the above equations, there exists
\[
x^T (A^T A - c^2 I) x = \sum_{i=1}^n c_i^2 (\lambda_i - c^2) > 0 \quad \forall x \neq 0,
\]
which leads to $\lambda_1 > c^2$. From (5.1), one has
\[
\rho \left( (A^T A)^{-1} \right) = \lambda_1^{-1} < 1/c^2 \text{ and } |A^{-1}| < c^{-1}.
\]
The proof is completed. \hfill \Box

**Lemma 5.3.** If the WSBDF3 discrete convolution kernels $w_{n-k}^{(n)}$ in (4.2) are positive definite, the DOC kernels $\theta_{n-k}^{(n)}$ defined in (4.6) are also positive definite. For any real sequence $\{\mu^k\}_{k=1}^n$, it holds that
\[
\sum_{k=1}^n \mu^k \sum_{j=1}^k \theta_{k-j}^{(k)} \mu^j \geq 0 \quad \text{for } n \geq 1.
\]
Proof. Let $\mu = (\mu^1, \mu^2, \cdots, \mu^n)^T \in \mathbb{R}^n$. We can check
\[
\sum_{k=1}^{n} \mu^k \sum_{j=1}^{k} \theta_{k-j}^{(k)} \mu^j = \mu^T \Theta \mu \quad \text{for } n \geq 1
\]
with the matrix $\Theta$ in (4.8).

According to Lemmas 4.3, 2.3 and 2.2, we know that the matrix $W$ is positive definite. Let $\forall \mu \in \mathbb{R}^n$, $\mu \neq 0$, it yields $\nu = W\mu \neq 0$. Then we have
\[
\nu^T W^{-1} \nu = \mu^T W^T W^{-1} W \mu = \mu^T W^T \mu > 0.
\]

The proof is completed. □

5.1. Stability analysis. Now we establish the stability for the WSBDF3 method (4.4).

Lemma 5.4. Let WSBDF3 kernels $u_{n-k}^{(n)}$ be defined in (4.2) with $W > c\Lambda^{-1}$. Then the discrete solution $u^n$ of WSBDF3 method (4.4) is unconditionally stable in the $L^2$ norm
\[
\|u^n\| \leq \|u^0\| + C \sqrt{\sum_{k=1}^{n} \tau_k \| \theta f^k + (1 - \theta) f^{k-1} \|^2} \leq \|u^0\| + C \max_{1 \leq k \leq n} \|f^k\|.
\]

Proof. Multiplying both sides of (4.4) by the DOC kernels $\theta_{k-j}^{(k)}$, and summing $j$ from 1 to $k$, we derive
\[
\sum_{j=1}^{k} \theta_{k-j}^{(k)} D_3 u^j - \sum_{j=1}^{k} \theta_{k-j}^{(k)} (\theta \Delta u^j + (1 - \theta) \Delta u^{j-1}) = \sum_{j=1}^{k} \theta_{k-j}^{(k)} (\theta f^j + (1 - \theta) f^{j-1}).
\]

According to (4.1) and (4.7), it yields
\[
\sum_{j=1}^{k} \theta_{k-j}^{(k)} D_3 u^j = \sum_{j=1}^{k} \theta_{k-j}^{(k)} \sum_{l=1}^{j} w_{j-l}^{(j)} \nabla \tau u^j = \sum_{j=1}^{k} \nabla \tau u^j \sum_{l=1}^{k} \theta_{k-j}^{(k)} w_{j-l}^{(j)} = \nabla \tau u^k \quad \text{for } k \geq 1.
\]

Hence, we have
\[
\nabla \tau u^k - \sum_{j=1}^{k} \theta_{k-j}^{(k)} (\theta \Delta u^j + (1 - \theta) \Delta u^{j-1}) = \sum_{j=1}^{k} \theta_{k-j}^{(k)} (\theta f^j + (1 - \theta) f^{j-1}).
\]

Making the inner product of (5.3) with $v^k = \theta u^k + (1 - \theta) u^{k-1}$, and summing the resulting equality from $k = 1$ to $n$, there exists
\[
\sum_{k=1}^{n} \langle \nabla \tau u^k, v^k \rangle + \sum_{k=1}^{n} \sum_{j=1}^{k} \theta_{k-j}^{(k)} (\theta \nabla u^j + (1 - \theta) \nabla u^{j-1}, \nabla v^k)
\]
\[
= \sum_{k=1}^{n} \sum_{j=1}^{k} \theta_{k-j}^{(k)} (\theta f^j + (1 - \theta) f^{j-1}, v^k), \quad n \geq 1.
\]
For the first term on the left hand, we have
\[
\sum_{k=1}^{n} (\nabla u^k, v^k) = \sum_{k=1}^{n} (u^k - u^{k-1}, \theta u^k + (1 - \theta) u^{k-1})
\]
\[
= \sum_{k=1}^{n} [(1 - \theta) (u^k - u^{k-1}, u^k + u^{k-1}) + (2\theta - 1) (u^k - u^{k-1}, u^k)]
\]
\[
\geq \sum_{k=1}^{n} \left[ (1 - \theta) \left( \|u^k\|^2 - \|u^{k-1}\|^2 \right) + \frac{2\theta - 1}{2} \left( \|u^k\|^2 - \|u^{k-1}\|^2 \right) \right]
\]
\[
= \frac{1}{2} \sum_{k=1}^{n} \left( \|u^k\|^2 - \|u^{k-1}\|^2 \right) = \frac{1}{2} \left( \|u^n\|^2 - \|u^0\|^2 \right),
\]
where the inequality \(2a(a - b) \geq a^2 - b^2\) has been used.

For the second term on the left hand, using Lemma 5.3, we obtain
\[
\sum_{k=1}^{n} \sum_{j=1}^{k} \theta_{k-j}^{(k)} \left( \theta \nabla u^j + (1 - \theta) \nabla u^{j-1}, \theta \nabla u^k + (1 - \theta) \nabla u^{k-1} \right) \geq 0.
\]

From (5.4), (5.5), (4.8), discrete Cauchy-Schwarz inequality and (5.1), it yields
\[
\|u^n\|^2 - \|u^0\|^2 \leq \frac{1}{2} \sum_{k=1}^{n} \sum_{j=1}^{k} \theta_{k-j}^{(k)} \left( \theta f^j + (1 - \theta) f^{j-1}, v^k \right) = 2 \int_{\Omega} V^T \Theta F dx
\]
\[
= 2 \int_{\Omega} \langle \Theta F, V \rangle dx = 2 \int_{\Omega} \langle W^{-1} F, V \rangle dx = 2 \int_{\Omega} \langle \mathcal{A}^{-1} \Lambda^{1/2} F, \Lambda^{1/2} V \rangle dx
\]
\[
\leq 2 \int_{\Omega} |\mathcal{A}^{-1}| \left| \Lambda^{1/2} F \right| \left| \Lambda^{1/2} V \right| dx
\]
with
\[
V = (v^1, v^2, \cdots, v^n)^T,
\]
\[
F = \left( \theta f^1 + (1 - \theta) f^0, \theta f^2 + (1 - \theta) f^1, \cdots, \theta f^n + (1 - \theta) f^{n-1} \right)^T.
\]

According to Lemmas 5.1, 5.2 and Cauchy-Schwarz inequality, we get
\[
\|u^n\|^2 - \|u^0\|^2 \leq C \int_{\Omega} \left| \Lambda^{1/2} F \right| \left| \Lambda^{1/2} V \right| dx \leq C \int_{\Omega} |\Lambda^{1/2} F|^2 dx \sqrt{\int_{\Omega} |\Lambda^{1/2} V|^2 dx}
\]
\[
= C \sqrt{\int_{\Omega} \sum_{k=1}^{n} \tau_k \left( \theta f^k + (1 - \theta) f^{k-1} \right)^2 dx} \sqrt{\int_{\Omega} \sum_{k=1}^{n} \tau_k (v^k)^2 dx}
\]
\[
= C \sqrt{\sum_{k=1}^{n} \tau_k \left( \theta f^k + (1 - \theta) f^{k-1} \right)^2} \sqrt{\sum_{k=1}^{n} \tau_k (v^k)^2}, \quad n \geq 1.
\]
Taking some integer \( n_1 (0 \leq n_1 \leq n) \) such that \( \| u^{n_1} \| = \max_{0 \leq k \leq n} \| u^k \| \). Taking \( n := n_1 \) in the above inequality, we get

\[
\| u^{n_1} \|^2 \leq \| u^0 \| \| u^{n_1} \| + C \| u^{n_1} \| \sum_{k=1}^{n_1} \tau_k \| \theta f^k + (1 - \theta) f^{k-1} \|^2.
\]

Hence, it yields

\[
(5.6) \quad \| u^n \| \leq \| u^0 \| + C \sum_{k=1}^{n} \tau_k \| \theta f^k + (1 - \theta) f^{k-1} \|^2 \leq \| u^0 \| + C \max_{1 \leq k \leq n} \| f^k \|.
\]

The proof is completed.

Theorem 5.1. Let WSBDF3 method be defined in (4.4) with the adjacent time-step ratio \( r_s \leq 1.771 \) for \( \theta = \frac{1}{2} \) and \( r_s \leq 1.405 \) for \( \theta = 1 \), respectively. Then the discrete solution \( u^n \) of WSBDF3 method is unconditionally stable in the \( L^2 \) norm

\[
\| u^n \| \leq \| u^0 \| + C \max_{1 \leq k \leq n} \| f^k \|, \quad n \geq 1.
\]

Proof. From Lemmas 5.4, 4.3, 3.5 and (4.9), (3.1), the desired results are obtained.

5.2. Convergence analysis. Now we establish the convergence analysis for the WSBDF3 method (4.4).

Lemma 5.5. For the consistency error \( \eta^j := \mathcal{D}_3 u(t_j) - \theta u'(t_j) - (1 - \theta) u'(t_{j-1}) \) for \( j \geq 1 \), it holds that

\[
\| \eta^1 \| \leq C \tau_1 \max_{0 < t \leq t_1} \| \partial_t u \|, \quad \| \eta^2 \| \leq C \left( \tau_1^2 + \tau_2 \right) \max_{0 < t \leq t_2} \| \partial_{tt} u \|,
\]

\[
\| \eta^j \| \leq C \left( \tau_j^3 + \tau_{j-1}^3 + \tau_{j-2}^3 \right) \max_{t_{j-3} \leq t \leq t_j} \| \partial_{ttt} u \| \quad \text{for} \quad j \geq 3.
\]

Proof. For simplicity, denote

\[
G_3^j = \int_{t_{j-1}}^{t_j} \| \partial_{tt} u \| dt \quad \text{and} \quad G_4^j = \int_{t_{j-1}}^{t_j} \| \partial_{ttt} u \| dt \quad \text{for} \quad j \geq 1.
\]

For the cases of \( j = 1 \) and \( j = 2 \), according to Lemma 4.1 in [6], we have

\[
\| \eta^1 \| \leq (2 - \theta) \tau_1 \max_{0 < t \leq t_1} \| \partial_t u \|,
\]

\[
\| \eta^2 \| \leq \frac{1 + 2 \tau r_0}{(1 + \tau_2)} G_3^1 + \frac{2(\theta - 1)}{2(1 + \tau_2)} \tau_1 G_3^1 \leq 2 \left( \tau_2^2 + \tau_1 \right) \max_{0 < t \leq t_2} \| \partial_{tt} u \|.
\]

For the case of \( j \geq 3 \), by using the Taylor’s expansion formula, it yields

\[
\eta^j = \frac{w_1^{(j)}}{6} \int_{t_{j-1}}^{t_j} (t - t_{j-1})^3 \partial_{ttt} u dt + \frac{w_2^{(j)}}{6} \int_{t_{j-2}}^{t_j} (t - t_{j-2})^2 \partial_{tt} u dt
\]

\[
- \frac{w_2^{(j)}}{6} \int_{t_{j-3}}^{t_j} (t - t_{j-3})^3 \partial_{ttt} u dt + \frac{1 - \theta}{2} \int_{t_{j-1}}^{t_j} (t - t_{j-1})^2 \partial_{tt} u dt.
\]
According to (4.2), the consistency error is bounded by
\[ \|\eta\| \leq C \left( \|w_0(j)\tau_3^3G_4^j - w_1(j)\tau_3^{-1}G_4^j - w_2(j)\tau_3\tau_2^{-2}G_4^j\right) \]
\[ \leq C \left( \tau_3^3 + \tau_3^{-1} + \tau_3\right) \max_{t_j \leq t \leq t_j+1} \|\partial_{ttt}u\|. \]
The proof is completed. \(\square\)

**Theorem 5.2.** Let \(u(t_n)\) and \(u^n\) be the solutions of the parabolic equation (1.1) and the WSBDF3 method (4.4), respectively. Then the time-discrete solution \(u^n\) is convergent in the \(L^2\) norm
\[ \|u(t_n) - u^n\| \leq C \max_{0 < t \leq t_1} \|\partial_t u\| \tau_1^{3/2} + C \max_{0 < t \leq t_2} \|\partial_{ttt}u\| \tau_2^{1/2} (\tau_1^2 + \tau_2^2) \]
\[ + C \max_{0 < t \leq T} \|\partial_{ttt}u\| \left( \sum_{k=3}^n \tau_k \right) \left( \tau_3^3 + \tau_3^{-1} + \tau_3\right)^{1/2} \]

**Proof.** Let \(e^n = u(t_n) - u^n\). From (1.1) and (4.4), we obtain
\[ D_3e^n - \theta \Delta e^n - (1 - \theta) \Delta e^{n-1} = D_3u(t_n) - \theta u'(t_n) - (1 - \theta) u'(t_{n-1}) = \eta^n, \quad n \geq 1. \]
According to (5.6), it yields
\[ \|e^n\| \leq C \sum_{k=1}^n \tau_k \|\eta^k\|^2 \leq C \left[ \|\tau_1^{1/2} \eta^1\|^2 + \|\tau_2^{1/2} \eta^2\|^2 + \sum_{k=3}^n \tau_k \|\eta^k\|^2 \right] \]
\[ \leq C \left[ \|\tau_1^{1/2} \eta^1\|^2 + \|\tau_2^{1/2} \eta^2\|^2 + \sum_{k=3}^n \tau_k \|\eta^k\|^2 \right]. \]
The desired result follows from Lemma 5.5 immediately. \(\square\)

6. **Numerical example**

We apply the WSBDF3 method (4.4) to the initial and boundary value problem (1.1) with \(\Omega = (-1,1)^2\) and \(T = 1\), subject to homogeneous Dirichlet boundary conditions. In space, we discretize by the spectral collocation method with the Chebyshev–Gauss–Lobatto points. We numerically verified the theoretical results including convergence orders in the discrete \(L^2\)-norm. In order to test the temporal error, we fix \(M_s = M_y = 20\); the spatial error is negligible since the spectral collocation method converges exponentially; see, e.g., [18, Theorem 4.4, §4.5.2].

**Example 6.1.** The initial value and the forcing term are chosen such that the exact solution of equation (1.1) is
\[ u(x,t) = (t^4 + 1)(1 - x^2)(1 - y^2), \quad -1 \leq x, y \leq 1, \ 0 \leq t \leq 1. \]
Here, we consider the arbitrary meshes with random time-steps \(\tau_k = T \epsilon_k / S\) for \(1 \leq k \leq N\), where \(S = \sum_{k=1}^N \epsilon_k\) and \(\epsilon_k \in (0,1)\) are random numbers subject to the uniform distribution [6, 16].

Table 6.1 shows the optimal convergence orders, which agrees with Theorem 5.2.
Table 6.1. The discrete $L^2$-norm errors and numerical convergence orders.

| $N$ |  $\theta = 1/2$ |  $\theta = 2/3$ |  $\theta = 1$ | $\max r_k$ | $\min r_k$ |
|-----|-----------------|-----------------|---------------|-----------|-----------|
| 20  | 9.890e-05       | 1.4312e-04      | 2.2243e-04    | 44.392    | 0.0405    |
| 40  | 1.1860e-05      | 3.0599e-05      | 1.6651e-05    | 3.1036    | 2.6076e-05 |
| 80  | 1.4898e-06      | 2.9929e-06      | 2.8863e-06    | 3.8311e-06| 2.7669    | 48.893    | 0.0121    |
| 160 | 1.9579e-07      | 2.9278e-07      | 2.8169e-07    | 4.3834e-07| 3.1276    | 76.033    | 0.0121    |

References

1. G. Akrivis, M. H. Chen, F. Yu, and Z. Zhou, *The energy technique for the six-step BDF method*, SIAM J. Numer. Anal. **59** (2021) 2449–2472.
2. J. Becker, *A second order backward difference method with variable steps for a parabolic problem*, BIT. **38** (1998) 644–662.
3. M. Calvo, T. Grande, and R. D. Grigorieff, *On the zero stability of the variable order variable stepsize BDF-formulas*, Numer. Math. **57** (1990) 151–167.
4. M. Calvo and R. D. Grigorieff, *Time discretisation of parabolic problems with the variable 3-step BDF*, BIT. **42** (2002) 689–701.
5. R. H. Chan and X. Q. Jin, *An Introduction to Iterative Toeplitz Solvers*, SIAM, Philadelphia, 2007.
6. M. H. Chen, F. Yu, and Q. D. Zhang, *Weighted and shifted BDF2 methods on variable grids*, arXiv:2108.02910.
7. W. Chen, X. Wang, Y. Yan, and Z. Zhang, *A second order BDF numerical scheme with variable steps for the Cahn-Hilliard equation*, SIAM J. Numer. Anal. **57** (2019) 495–525.
8. M. Crouzeix and F. J. Lisbona, *The convergence of variable-stepsize, variable formula, multistep methods*, SIAM J. Numer. Anal. **21** (1984) 512–534.
9. C. W. Cryer, *A new class of highly-stable methods: $A_0$-stable methods*, BIT. **2** (1973) 153–159.
10. E. Emmrich, *Stability and error of the variable two-step BDF for semilinear parabolic problems*, J. Appl. Math. Comput. **19** (2005) 33–55.
11. R. D. Grigorieff, *Stability of multistep-methods on variable grids*, Numer. Math. **42** (1983) 359–377.
12. R. D. Grigorieff and P. J. Paeslame, *On the zero-stability of the 3-step BDF-formula on nonuniform grids*, BIT. **24** (1984) 85–91.
13. N. Guglielmi and M. Zennaro, *On the zero-stability of variable stepsize multistep methods: the spectral radius approach*, Numer. Math. **88** (2001) 445–458.
14. R. J. Leveque, *Finite difference methods for ordinary and partial differential equations*, SIAM, Washington, 2007.
15. Q. Y. Li and J. D. Xie, *A linear multistep method for solving stiff ordinary differential equations*, J. Tsinghua Univ. **31** (1991) 1–11.
16. H. Liao and Z. Zhang, *Analysis of adaptive BDF2 scheme for diffusion equations*, Math. Comp. **90** (2021) 1207–1226.
17. A. Quarteroni, R. Sacco, and F. Saleri, *Numerical Mathematics, 2nd ed*, Springer, 2007.
18. J. Shen, T. Tang, and L. Wang, *Spectral Methods: Algorithms, Analysis and Applications*, Springer-Verlag, Berlin, 2011.
19. G. Söderlind, I. Fekete, and I. Faragó, *On the zero-stability of multistep methods on smooth nonuniform grids*, BIT. **58** (2018) 1125–1143.
20. D. Wang and S. J. Ruuth, *Variable step-size implicit-explicit linear multistep methods for time-dependent partial differential equations*, J. Comput. Math. **26** (2008) 838–855.
