

THE ENERGY TECHNIQUE FOR THE SIX-STEP BDF METHOD*

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Abstract. In combination with the Grenander–Szegő theorem, we observe that a relaxed positivity condition on multipliers, milder than the basic requirement of the Nevanlinna–Odeh multipliers that the sum of the absolute values of their components is strictly less than 1, makes the energy technique applicable to the stability analysis of BDF methods for parabolic equations with selfadjoint elliptic part. This is particularly useful for the six-step BDF method for which we show that no Nevanlinna–Odeh multipliers exist. We introduce multipliers satisfying the positivity property for the six-step BDF method and establish stability of the method for parabolic equations.

Key words. Six-step BDF method, multipliers, parabolic equations, stability estimate, energy technique.

AMS subject classifications. Primary 65M12, 65M60; Secondary 65L06

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

$$(1.1) \quad \begin{cases} u'(t) + Au(t) = f(t), & 0 < t < T, \\ u(0) = u^0, \end{cases}$$

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

We consider the q -step backward difference formula (BDF) method, generated by the polynomials α and β ,

$$(1.2) \quad \alpha(\zeta) = \sum_{j=1}^q \frac{1}{j} \zeta^{q-j} (\zeta - 1)^j = \sum_{j=0}^q \alpha_j \zeta^j, \quad \beta(\zeta) = \zeta^q.$$

The BDF methods are $A(\vartheta_q)$ -stable with $\vartheta_1 = \vartheta_2 = 90^\circ$, $\vartheta_3 \approx 86.03^\circ$, $\vartheta_4 \approx 73.35^\circ$, $\vartheta_5 \approx 51.84^\circ$ and $\vartheta_6 \approx 17.84^\circ$; see [13, Section V.2]. Nørsett established a criterion for $A(\vartheta)$ -stability in [22] and numerically computed the approximations $\vartheta_3^N \approx 88.45^\circ$, $\vartheta_4^N \approx 73.23333^\circ$, $\vartheta_5^N \approx 51.83333^\circ$ and $\vartheta_6^N \approx 18.78333^\circ$. Exact values of ϑ_q , $q = 3, 4, 5, 6$, are given in [5]; see also [19], [12]. The order of the q -step method is q .

Let $N \in \mathbb{N}$, $\tau := T/N$ be the time step, and $t^n := n\tau$, $n = 0, \dots, N$, be a uniform partition of the interval $[0, T]$. We recursively define a sequence of approximations u^m to the nodal

*Received by the editors January 19, 2021, accepted for publication (in revised form) June 18, 2021.

Funding: The research of M. Chen and F. Yu is partially supported by NSFC 11601206, and the research of Z. Zhou is supported by Hong Kong RGC grant (No. 25300818).

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values $u(t^m)$ of the exact solution by the q -step BDF method,

$$(1.3) \quad \sum_{i=0}^q \alpha_i u^{n+i} + \tau Au^{n+q} = \tau f^{n+q}, \quad n = 0, \dots, N - q,$$

with $f^m := f(t^m)$, assuming that starting approximations u^0, \dots, u^{q-1} are given.

Let $|\cdot|$ denote the norm on H induced by the inner product (\cdot, \cdot) , and introduce on $V, V := D(A^{1/2})$, the norm $\|\cdot\|$ by $\|v\| := |A^{1/2}v|$. We identify H with its dual, and denote by V' the dual of V , and by $\|\cdot\|_*$ the dual norm on $V', \|v\|_* = |A^{-1/2}v|$. We shall use the notation (\cdot, \cdot) also for the antiduality pairing between V' and V .

In view of the positivity of the coefficient α_q , the Lax–Milgram lemma ensures existence and uniqueness of the BDF approximations.

Stability of the A-stable one- and two-step BDF methods (1.3) can be easily established by the energy technique. The powerful Nevanlinna–Odeh multiplier approach extends the applicability of the energy method to the non A-stable three-, four- and five-step BDF methods. In contrast, as we shall see, no Nevanlinna–Odeh multipliers exist for the six-step BDF method. Here, we show that, in combination with the Grenander–Szegő theorem, see Lemma 3.2, the energy technique is applicable even with multipliers satisfying milder requirements than Nevanlinna–Odeh multipliers. We introduce such multipliers for the six-step BDF method and establish stability estimates by the energy technique.

Several stability techniques have been developed for BDF methods, each one with its own merits. The main characteristics that make the energy technique so powerful are its simplicity and flexibility. In particular, the energy technique can be easily combined with other stability techniques such as the discrete maximal parabolic L^p -regularity, and, depending on the choice of the test functions, it leads to several stability estimates. We refer to [16] for the maximal parabolic regularity property of the BDF methods and to [6] for an efficient combination of the discrete maximal parabolic regularity and the energy technique for BDF methods of order up to 5 in the case of the discretization of quasilinear parabolic equations. The energy technique has proven particularly useful in recent years in the analyses of various variants of BDF methods of order up to 5, such as fully implicit, linearly implicit or implicit–explicit, for a series of nonlinear equations of parabolic type; cf., e.g., [20, 7, 1, 4, 6, 17, 3].

Stability conditions involving multipliers are familiar for feedback systems from control theory; see, e.g., [25] and references therein.

An outline of the paper is as follows: In Section 2, we relax the requirements on the multipliers for BDF methods and present multipliers for the six-step BDF method. In Section 3, we use a new multiplier in combination with the Grenander–Szegő theorem and prove stability of the six-step BDF method for the initial value problem (1.1) as well as for nonautonomous parabolic equations. In Section 4, we present some numerical results and compare the six-step BDF method with two Runge–Kutta methods of similar order, namely the three-stage Radau IIA and Gauss methods.

2. Multipliers for the six-step BDF method. Multipliers for the three-, four- and five-step BDF methods were introduced by Nevanlinna and Odeh already in 1981, see [21], to make the energy technique applicable to the stability analysis of these methods for parabolic equations; no multipliers are required for the A-stable one- and two-step BDF methods. The multiplier technique became widely known and popular after its first actual application to the stability analysis for parabolic equations by Lubich, Mansour, and Venkataraman in 2013; see [20].

The multiplier technique hinges on the celebrated equivalence of A- and G-stability for multistep methods by Dahlquist; see [11].

Lemma 2.1 ([11]; see also [8] and [13, Section V.6]). *Let $\alpha(\zeta) = \alpha_q \zeta^q + \dots + \alpha_0$ and $\kappa(\zeta) = \kappa_q \zeta^q + \dots + \kappa_0$ be polynomials, with real coefficients, of degree at most q (and at least one of them of degree q) that have no common divisor. Let (\cdot, \cdot) be a real inner product with associated norm $|\cdot|$. If*

$$(A) \quad \operatorname{Re} \frac{\alpha(\zeta)}{\kappa(\zeta)} > 0 \quad \text{for } |\zeta| > 1,$$

then there exists a positive definite symmetric matrix $G = (g_{ij}) \in \mathbb{R}^{q,q}$ and real $\delta_0, \dots, \delta_q$ such that for v^0, \dots, v^q in the inner product space,

$$(G) \quad \left(\sum_{i=0}^q \alpha_i v^i, \sum_{j=0}^q \kappa_j v^j \right) = \sum_{i,j=1}^q g_{ij} (v^i, v^j) - \sum_{i,j=1}^q g_{ij} (v^{i-1}, v^{j-1}) + \left| \sum_{i=0}^q \delta_i v^i \right|^2.$$

Notice that we here consider real spaces for simplicity of notation; in the case of a complex inner product, (G) is still valid with the term on its left-hand side replaced by its real part.

Definition 2.2 (Multipliers and Nevanlinna–Odeh multipliers). Let α be the generating polynomial of the q -step BDF method defined in (1.2). Consider a q -tuple (μ_1, \dots, μ_q) of real numbers such that with the given α and, abusing notation a little bit, $\mu(\zeta) := \zeta^q - \mu_1 \zeta^{q-1} - \dots - \mu_q$, the pair (α, μ) satisfies the A-stability condition (A), with $\kappa(\zeta)$ replaced by $\mu(\zeta)$, and, in addition, the polynomials α and μ have no common divisor. Then, we call (μ_1, \dots, μ_q) *Nevanlinna–Odeh multiplier* for the q -step BDF method if

$$(P1) \quad 1 - |\mu_1| - \dots - |\mu_q| > 0,$$

and simply *multiplier* if it satisfies the *positivity* property

$$(P2) \quad 1 - \mu_1 \cos x - \dots - \mu_q \cos(qx) > 0 \quad \forall x \in \mathbb{R}.$$

Notice that, with the notation of this definition, (A) and (G), respectively, mean that the q -step scheme described by the parameters $\alpha_q, \dots, \alpha_0, 1, -\mu_1, \dots, -\mu_q$ and the corresponding one-leg method are A- and G-stable, respectively. Of course, these are necessarily low order methods but this is irrelevant here; we do not compute with them; we only use them to establish stability of the q -step BDF method.

Optimal Nevanlinna–Odeh multipliers, i.e., the ones with minimal $|\mu_1| + \dots + |\mu_q|$, for the three-, four- and five-step BDF methods, were given in [4].

Some comments on the requirements in Definition 2.2 and their role in the stability analysis are in order. The essence of the positivity property (P2) is that, in combination with the Grenander–Szegő theorem, it ensures that symmetric band Toeplitz matrices $T = (t_{ij})_{i,j=1,\dots,m}$, of bandwidth $2q + 1$ and dimension $m \geq 2q + 1$, with entries $t_{ij} = t_{i-j}$,

$$(2.1) \quad t_0 = 1 - \varepsilon, \quad t_i = \mu_i/2, \quad i = 1, \dots, q, \quad t_i = 0, \quad i = q + 1, \dots, m - 1,$$

are, for sufficiently small ε , positive definite; see Section 3 for the application of this property, with a concrete multiplier, for the case of the six-step BDF method. To prove stability of the method by the energy technique, we test (1.3) by $u^{n+q} - \mu_1 u^{n+q-1} - \dots - \mu_q u^n$ and obtain

$$(2.2) \quad \left(\sum_{i=0}^q \alpha_i u^{n+i}, u^{n+q} - \sum_{j=1}^q \mu_j u^{n+q-j} \right) + \tau A_{n+q} = \tau F_{n+q},$$

$n = 0, \dots, N - q$, with

$$(2.3) \quad A_{n+q} := \left(Au^{n+q}, u^{n+q} - \sum_{j=1}^q \mu_j u^{n+q-j} \right) \quad \text{and} \quad F_{n+q} := \left(f^{n+q}, u^{n+q} - \sum_{j=1}^q \mu_j u^{n+q-j} \right).$$

The term F_{n+q} in (2.2) can be easily estimated from above via elementary inequalities. The first term on the left-hand side of (2.2) can be estimated from below using (G); this is the motivation for the requirement (A). Which one of the two positivity conditions, (P1) or (P2), enters into the stability analysis, depends on the way we handle the second term on the left-hand side of (2.2), i.e., A_{n+q} . In the standard approach, we estimate A_{n+q} from below at every time level and subsequently sum over n ; then, requirement (P1) is crucial; cf., e.g., [7], [1], [4]. Instead, in the proposed here approach, we sum over n and subsequently estimate the sum $A_q + \dots + A_m$, $m \leq N$, from below; in this way, it turns out that the relaxed positivity condition (P2) suffices. In the latter approach, the positive definiteness of symmetric band Toeplitz matrices T , of any dimension $m \geq 2q + 1$, with entries given in (2.1), plays a key role.

It is well known that the A-stability property (A) for a multiplier for the q -step BDF method implies

$$|\mu_1| + \dots + |\mu_q| \geq \cos \vartheta_q;$$

see [21]. In particular, for the six-step BDF method this means that $|\mu_1| + \dots + |\mu_6| \geq 0.9516169$. Actually, as we shall see, no Nevanlinna–Odeh multiplier exists for the six-step BDF method; see Remark 2.6. This was the motivation for our relaxation on the requirements for multipliers. Fortunately, the relaxed positivity condition (P2) leads to a positive result.

Proposition 2.3 (A multiplier for the six-step BDF method). *The set of numbers*

$$(2.4) \quad \mu_1 = \frac{13}{9}, \quad \mu_2 = -\frac{25}{36}, \quad \mu_3 = \frac{1}{9}, \quad \mu_4 = \mu_5 = \mu_6 = 0,$$

is a multiplier for the six-step BDF method.

Proof. The proof consists of two parts; we first prove the A-stability property (A) and subsequently the positivity property (P2).

A-stability property (A). The corresponding polynomial μ is

$$(2.5) \quad \begin{aligned} \mu(\zeta) &= \zeta^3 \left(\zeta - \frac{1}{2} \right)^2 \left(\zeta - \frac{4}{9} \right) = \zeta^6 - \frac{13}{9} \zeta^5 + \frac{25}{36} \zeta^4 - \frac{1}{9} \zeta^3 \\ &= \frac{1}{36} \zeta^3 (36\zeta^3 - 52\zeta^2 + 25\zeta - 4). \end{aligned}$$

We recall the generating polynomial α of the six-step BDF method,

$$60\alpha(\zeta) = 147\zeta^6 - 360\zeta^5 + 450\zeta^4 - 400\zeta^3 + 225\zeta^2 - 72\zeta + 10.$$

First, $\alpha(0) = 1/6$, $\alpha(1/2) = -37/3840$ and $\alpha(4/9) = -0.003730423508913$, whence the polynomials α and μ have no common divisor.

Now, $\alpha(z)/\mu(z)$ is holomorphic outside the unit disk in the complex plane, and

$$\lim_{|z| \rightarrow \infty} \frac{\alpha(z)}{\mu(z)} = \alpha_6 = \frac{147}{60} > 0.$$

Therefore, according to the maximum principle for harmonic functions, the A-stability property (A) is equivalent to

$$\operatorname{Re} \frac{\alpha(\zeta)}{\mu(\zeta)} \geq 0 \quad \forall \zeta \in \mathcal{K},$$

with \mathcal{K} the unit circle in the complex plane, $\mathcal{K} := \{\zeta \in \mathbb{C} : |\zeta| = 1\}$, i.e., equivalent to

$$(2.6) \quad \operatorname{Re} [\alpha(e^{i\varphi})\mu(e^{-i\varphi})] \geq 0 \quad \forall \varphi \in \mathbb{R}.$$

In view of (2.5), the desired property (2.6) takes the form

$$(2.7) \quad \operatorname{Re} [60\alpha(e^{i\varphi})e^{-i3\varphi}(36e^{-i3\varphi} - 52e^{-i2\varphi} + 25e^{-i\varphi} - 4)] \geq 0 \quad \forall \varphi \in \mathbb{R}.$$

Now, it is easily seen that

$$\begin{aligned} 60\alpha(e^{i\varphi})e^{-i3\varphi} &= [157 \cos(3\varphi) - 432 \cos(2\varphi) + 675 \cos \varphi - 400] \\ &\quad + i[137 \sin(3\varphi) - 288 \sin(2\varphi) + 225 \sin \varphi]. \end{aligned}$$

With $x := \cos \varphi$, recalling the elementary trigonometric identities

$$\cos(2\varphi) = 2x^2 - 1, \quad \cos(3\varphi) = 4x^3 - 3x, \quad \sin(2\varphi) = 2x \sin \varphi, \quad \sin(3\varphi) = (4x^2 - 1) \sin \varphi,$$

we easily see that

$$(2.8) \quad 60\alpha(e^{i\varphi})e^{-i3\varphi} = 4(1-x)(8 + 59x - 157x^2) + i4(137x^2 - 144x + 22) \sin \varphi.$$

Notice that the factor $1-x$ in the real part of $\alpha(e^{i\varphi})e^{-i3\varphi}$ is due to the fact that $\alpha(1) = 0$. Similarly,

$$\begin{aligned} 36e^{-i3\varphi} - 52e^{-i2\varphi} + 25e^{-i\varphi} - 4 &= [36 \cos(3\varphi) - 52 \cos(2\varphi) + 25 \cos \varphi - 4] \\ &\quad - i[36 \sin(3\varphi) - 52 \sin(2\varphi) + 25 \sin \varphi] \end{aligned}$$

and

$$(2.9) \quad \begin{aligned} 36e^{-i3\varphi} - 52e^{-i2\varphi} + 25e^{-i\varphi} - 4 &= (144x^3 - 104x^2 - 83x + 48) \\ &\quad - i(144x^2 - 104x - 11) \sin \varphi. \end{aligned}$$

In view of (2.8) and (2.9), the desired property (2.7) can be written in the form

$$(2.10) \quad 4(1-x)P(x) \geq 0 \quad \forall x \in [-1, 1]$$

with

$$\begin{aligned} P(x) &:= (8 + 59x - 157x^2)(144x^3 - 104x^2 - 83x + 48) \\ &\quad + (1+x)(137x^2 - 144x + 22)(144x^2 - 104x - 11), \end{aligned}$$

i.e.,

$$(2.11) \quad P(x) = 2(71 + 611x + 1334x^2 - 5150x^3 + 4784x^4 - 1440x^5).$$

It is now easy to see that P is positive in the interval $[-1, 1]$, and thus that (2.7) is valid. First, the quadratic polynomial $71 + 611x + 1334x^2$ is positive for all real x , since it does

not have real roots. All other terms are positive for negative x , whence $P(x)$ is positive for negative x . Furthermore, for $0 \leq x \leq 1$, we obviously have $71 + 611x \geq 682x^2$, and can estimate $P(x)$ from below as follows

$$\begin{aligned} P(x) &\geq 2x^2(2016 - 5150x + 4784x^2 - 1440x^3) \\ &= 2x^2[(2016 - 5150x + 3344x^2) + 1440x^2(1 - x)]. \end{aligned}$$

Again, the quadratic polynomial $2016 - 5150x + 3344x^2$ is positive for all real x , and the positivity of $P(x)$ follows. See also Figure 2.1.

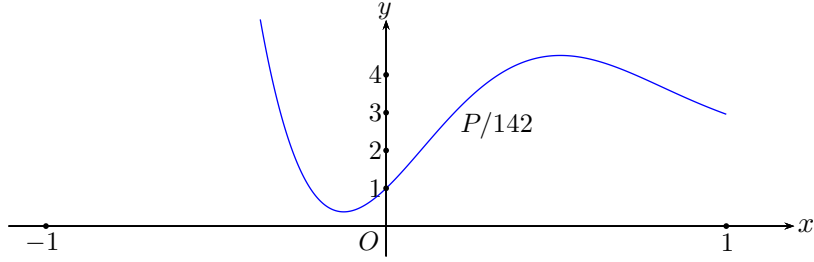


Figure 2.1. The graph of polynomial $P/142$ of (2.11) in the interval $[-0.37, 1]$.

Positivity property (P2). Here, we prove the desired positivity property (P2) for the multiplier (2.4). Actually, since in the stability analysis we will use the value $\varepsilon = 1/32$ in (2.1), to avoid repetitions, we shall directly prove that the function in (P2) for the multiplier (2.4) is bounded from below by $1/32$. To this end, we subtract $1/32$ from the corresponding expression, and shall show that the function g ,

$$(2.12) \quad g(s) := \frac{31}{32} - \frac{13}{9} \cos s + \frac{25}{36} \cos(2s) - \frac{1}{9} \cos(3s), \quad s \in \mathbb{R},$$

is positive. Now, elementary trigonometric identities lead to the following form of g

$$g(s) = -\frac{4}{9} \cos^3 s + \frac{25}{18} \cos^2 s - \frac{10}{9} \cos s + \frac{79}{288}.$$

Hence, we consider the polynomial p ,

$$(2.13) \quad p(x) := -\frac{4}{9}x^3 + \frac{25}{18}x^2 - \frac{10}{9}x + \frac{79}{288}, \quad x \in [-1, 1].$$

It is easily seen that p attains its minimum in $[-1, 1]$ at $x^* = (25 - \sqrt{145})/24$ and

$$p(x^*) = 0.009321552602567 > 0.$$

Therefore, g is indeed positive; in particular, the desired positivity property (P2) is satisfied. See also Figure 2.2. ■

2.1. On the conditions (P2) and (P1). We briefly comment on the discrepancy between the positivity conditions (P2) and (P1). Obviously, (P1) implies (P2).

Let $S_q \subset \mathbb{R}^q$ denote the region of the points (μ_1, \dots, μ_q) satisfying the positivity condition (P2). Since (P1) and (P2) are obviously equivalent for q -tuples (μ_1, \dots, μ_q) with only one

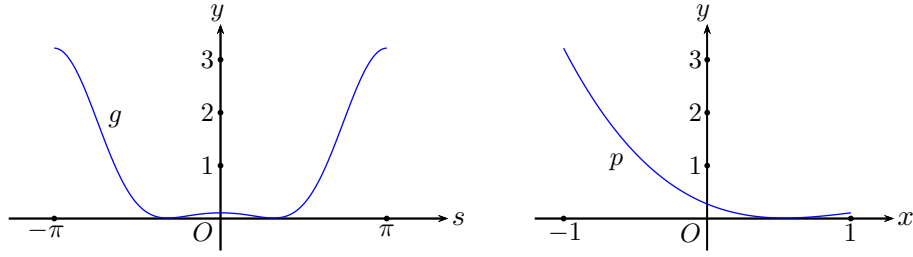


Figure 2.2. The graphs of the function g and the polynomial p of (2.12) and (2.13).

nonvanishing component, the intersection of S_q with each coordinate axis is an interval of the form $(-1, 1)$.

Let us next focus on the instrumental case of S_2 , that is, of the intersection of S_q with the $\mu_1\mu_2$ plane, i.e., consider the set of points $(\mu_1, \dots, \mu_q) \in S_q$ with $\mu_3 = \dots = \mu_q = 0$. Then, the positivity condition reads

$$(2.14) \quad p(x) := 1 - \mu_1 x - \mu_2(2x^2 - 1) > 0, \quad x \in [-1, 1].$$

For $\mu_2 = 0$, this condition is satisfied if and only if $|\mu_1| < 1$. For nonvanishing μ_2 , the derivative of p vanishes at $x^* = -\mu_1/(4\mu_2)$ and

$$(2.15) \quad p(x^*) = 1 + \mu_2 + \frac{1}{8} \frac{\mu_1^2}{\mu_2}.$$

For positive μ_2 , this is a positive global maximum of p . Therefore, in this case (2.14) is satisfied if and only if $p(-1)$ and $p(1)$ are positive, whence

$$(2.16) \quad \mu_2 < 1 - |\mu_1|.$$

For negative μ_2 , the expression in (2.15) is a global minimum of p . Now, we distinguish two subcases. If $|\mu_2| \leq |\mu_1|/4$, then the minimum is attained at a point $|x^*| \geq 1$, whence (2.16) suffices for (2.14). If, on the other hand, $|x^*| < 1$, then (2.14) is satisfied if and only if the expression on the right-hand side of (2.15) is positive, i.e.,

$$4\left(\mu_2 + \frac{1}{2}\right)^2 + \frac{1}{2}\mu_1^2 < 1;$$

that is, (μ_1, μ_2) lies in the interior of an ellipse. Summarizing, (2.14) is satisfied if and only if (μ_1, μ_2) lie in the region

$$S_2 = \left\{ (\mu_1, \mu_2) : -\frac{|\mu_1|}{4} \leq \mu_2 < 1 - |\mu_1| \right\} \\ \cup \left\{ (\mu_1, \mu_2) : 4\left(\mu_2 + \frac{1}{2}\right)^2 + \frac{1}{2}\mu_1^2 < 1 \text{ and } |\mu_2| > \frac{|\mu_1|}{4} \right\}.$$

Notice that the lines $\mu_2 = \pm(1 - \mu_1)$ are tangent to the ellipse at their intersection points with the lines $\mu_2 = \mp\mu_1/4$, respectively, i.e., at the points $(\pm 4/3, -1/3)$. This is, of course, due to the fact that for these values the global minimum in (2.15) is attained at the points $x^* = \pm 1$. Therefore, the intersection S_2 of S_q with the $\mu_1\mu_2$ plane is the union of two overlapping simple sets, a triangle and an ellipse,

$$(2.17) \quad S_2 = \left\{ (\mu_1, \mu_2) : -\frac{1}{3} \leq \mu_2 < 1 - |\mu_1| \right\} \cup \left\{ (\mu_1, \mu_2) : 4\left(\mu_2 + \frac{1}{2}\right)^2 + \frac{1}{2}\mu_1^2 < 1 \right\};$$

see Figure 2.3, right. Notice, in particular, that

$$(2.18) \quad |\mu_1| < \sqrt{2} \quad \text{and} \quad |\mu_2| < 1.$$

Replacing x by $x/2$ and by $x/3$, respectively, in the positivity condition (P2), it is obvious that the intersection of S_q with the $\mu_2\mu_4$ plane, for $q \geq 4$, and with the $\mu_3\mu_6$ plane, for $q = 6$, respectively, is of the form (2.17) with (μ_1, μ_2) replaced by (μ_2, μ_4) and by (μ_3, μ_6) , respectively.

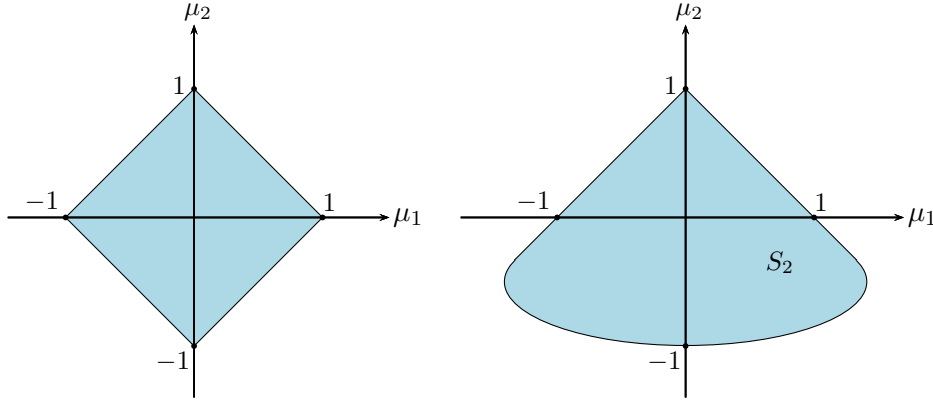


Figure 2.3. Illustration of the conditions (P1) and (P2), left and right, respectively, for $\mu_3 = \dots = \mu_6 = 0$; cf. (2.17).

2.2. On the construction of multipliers. In this part, we describe some necessary conditions of multipliers for the six-step BDF method satisfying the A-stability condition (A) and the relaxed positivity condition (P2). To begin with, we show that no multiplier with $\mu_3 = \dots = \mu_6 = 0$ exists.

Proposition 2.4. *There is no multiplier for the six-step BDF method with $\mu_3 = \dots = \mu_6 = 0$, satisfying (A) and (P2).*

Proof. The positivity condition (P2) is satisfied if and only if

$$1 - \mu_1 x - \mu_2(2x^2 - 1) > 0 \quad \forall x \in [-1, 1];$$

see (2.14). The A-stability condition (A) is in this case equivalent to (2.10) with

$$(2.19) \quad \begin{aligned} P(x) = & (8 + 59x - 157x^2)(4x^3 - \mu_1(2x^2 - 1) - 3x - \mu_2x) \\ & + (1 + x)(137x^2 - 144x + 22)(4x^2 - 2\mu_1x - \mu_2 - 1). \end{aligned}$$

First, the estimate $|\mu_1| < \sqrt{2}$ in (2.18) and the nonnegativity of

$$P(-4/25) = -41.65312\mu_2 + 7.86979\mu_1 - 39.13478$$

lead to the estimate

$$(2.20) \quad \mu_2 < \frac{7.86979\sqrt{2} - 39.13478}{41.65312} < -0.672343782385853.$$

On the other hand, for $\mu_2 < -0.672343782385853$, we have $|\mu_2| > |\mu_1|/4$, and thus (μ_1, μ_2) must lie in the interior of the ellipse in (2.17). Now, $P(0.99) = a\mu_2 + b\mu_1 + c$ with

$$a = \frac{2086460708677967}{35184372088832}, \quad b = \frac{1053766469372221}{35184372088832}, \quad c = \frac{9685378027}{109951162777600},$$

and the intersection points of the line $P(0.99) = 0$ and the ellipse $4(\mu_2 + 1/2)^2 + \mu_1^2/2 = 1$ are

$$(2.21) \quad \begin{cases} A = (2.941186035762484 \cdot 10^{-6}, -1.08131109678632 \cdot 10^{-12}), \\ B = (1.328818676149621, -0.671118740185537). \end{cases}$$

It is easily seen that $P(0.99)$ is nonnegative only in the part of the interior of the ellipse to the right of the segment AB ; cf. Figure 2.4. Therefore, $P(0.99) \geq 0$ implies

$$\mu_2 \geq -0.671118740185537.$$

This together with (2.20) leads to a contradiction; hence, no multiplier of the form $(\mu_1, \mu_2, 0, \dots, 0)$ exists for the six-step BDF method. ■

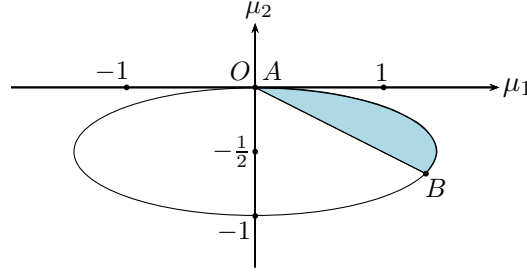


Figure 2.4. Out of the interior points (μ_1, μ_2) of the ellipse, $P(0.99)$, see (2.19), is nonnegative only in the blue region; in the blue region, $\mu_2 \geq -0.671118740185535$. The points A and B are given in (2.21). The points A and $O = (0, 0)$ are visually not distinguishable.

Our next attempt was to seek a multiplier for the six-step BDF method with $\mu_4 = \mu_5 = \mu_6 = 0$. In this case, the A-stability condition (A) and the positivity condition (P2) lead, respectively, to the conditions

$$(2.22) \quad \begin{aligned} P(x) = & (8 + 59x - 157x^2)(4x^3 - \mu_1(2x^2 - 1) - 3x - \mu_2x - \mu_3) \\ & + (1 + x)(137x^2 - 144x + 22)(4x^2 - 2\mu_1x - \mu_2 - 1) \geq 0 \end{aligned}$$

for all $x \in [-1, 1]$, and

$$(2.23) \quad g(x) := 1 - \mu_1 \cos x - \mu_2 \cos(2x) - \mu_3 \cos(3x) > 0 \quad \forall x \in \mathbb{R}.$$

Necessary conditions for (2.22) and (2.23) could be derived by evaluating P and g at certain points. For instance, we claim the following necessary condition, which helps us to construct multipliers.

Proposition 2.5. *If $(\mu_1, \mu_2, \mu_3, 0, 0, 0)$ is a multiplier of the six-step BDF method, then there holds*

$$0.41990729 < \mu_1 < \sqrt{3}, \quad -1 < \mu_2 < -0.58852878, \quad 0 < \mu_3 < 1, \quad |\mu_1| + |\mu_2| + |\mu_3| > 1.$$

Proof. First, $|\mu_2| < 1$ follows immediately from the positivity of $g(\pi/2)$ and of $g(0)$ and $g(\pi)$. Furthermore,

$$2g(2\pi/3) + g(0) = 3(1 - \mu_3) \quad \text{and} \quad 2g(\pi/3) + g(\pi) = 3(1 + \mu_3),$$

whence $|\mu_3| < 1$. In view of

$$g(\pi/6) = \frac{1}{2}(-\sqrt{3}\mu_1 - \mu_2 + 2) \quad \text{and} \quad g(5\pi/6) = \frac{1}{2}(\sqrt{3}\mu_1 - \mu_2 + 2),$$

we have $\sqrt{3}|\mu_1| < 2 - \mu_2$, and, in combination with $\mu_2 > -1$, infer that $|\mu_1| < \sqrt{3}$.

Up to this point, we did not use the nonnegativity of P . Now we check $P(0) \geq 0$, i.e.,

$$P(0) = 2[4(\mu_1 - \mu_3) - 11(1 + \mu_2)] \geq 0.$$

Since $1 + \mu_2 > 0$, we infer that $\mu_3 < \mu_1$. Furthermore, since $\mu_1 < \sqrt{3}$ and $|\mu_3| < 1$,

$$11\mu_2 < 4(\sqrt{3} + 1) - 11 < -0.07179, \quad \text{whence} \quad \mu_2 < -0.65263636 \cdot 10^{-2}.$$

Meanwhile, since $274/625 + 1154\mu_2/25 < 0$, the nonnegativity of

$$P(0.8) = \frac{274}{625} + \frac{1154}{25}\mu_2 + \frac{3572}{125}\mu_1 + \frac{1132}{25}\mu_3$$

yields $3572\mu_1/125 + 1132\mu_3/25 > 0$, which together with $\mu_3 < \mu_1$ leads to

$$\frac{3572}{125}\mu_1 + \frac{1132}{25}\mu_1 > \frac{3572}{125}\mu_1 + \frac{1132}{25}\mu_3 > 0,$$

i.e., $\mu_1 > 0$. Therefore, we arrive at

$$0 < \mu_1 < \sqrt{3}, \quad -1 < \mu_2 < -0.65263636 \cdot 10^{-2} \quad \text{and} \quad 0 < |\mu_3| < 1.$$

Next, we prove $\mu_3 > 0$ by contradiction. If $\mu_3 \leq 0$, then the positivity of $g(\pi/4)$ yields

$$g(\pi/4) = 1 - \frac{\sqrt{2}}{2}(\mu_1 - \mu_3) > 0 \implies \mu_1 < \sqrt{2}.$$

This and the nonnegativity of $P(-4/25)$ imply $\mu_2 < -0.672$. Then, we can derive a lower bound $\mu_1 > 1.3426$ by examining $P(0.999) \geq 0$. However, with $\mu_1 > 1.3426$, $\mu_2 < -0.672$ and $\mu_3 \leq 0$, it is easy to observe that

$$2g(\pi/3) = -\mu_1 + \mu_2 + 2\mu_3 + 2 \leq -1.3426 - 0.672 + 2 < -0.0146,$$

which violates the positivity condition (2.23). Therefore, we conclude that $\mu_3 > 0$.

Moreover, from $\mu_1 < \sqrt{3}$, $\mu_3 > 0$ and the nonnegativity of

$$P(-66/625) = 7.33518936\mu_1 - 34.64182239\mu_2 - 0.01883648\mu_3 - 33.09263039,$$

we infer that

$$\mu_2 < \frac{7.33518936\sqrt{3} - 33.09263039}{34.64182239} < -0.58852878.$$

Then, the nonnegativity of $P(27/125)$ yields $\mu_1 > 0.41990729$. Thus, we arrive at

$$0.41990729 < \mu_1 < \sqrt{3}, \quad -1 < \mu_2 < -0.58852878 \quad \text{and} \quad 0 < \mu_3 < 1.$$

Finally, the property $|\mu_1| + |\mu_2| + |\mu_3| > 1$ is a special case of the more general result of the next Remark. ■

Remark 2.6 (Nonexistence of Nevanlinna–Odeh multipliers for the six-step BDF method). The multiplier (2.4) is not unique. In general, the A-stability condition (A) and the positivity condition (P2) lead to the conditions

$$\begin{aligned} P(x) = & (-80x^5 + 208x^4 - 122x^3 - 82x^2 + 98x - 22) \\ & + (40x^4 - 104x^3 + 71x^2 + 15x + 8)\mu_1 \\ & + (20x^3 - 52x^2 + 114x - 22)\mu_2 - (8 + 59x - 157x^2)\mu_3 \\ & + (294x^3 - 66x^2 - 130x + 22)\mu_4 + (588x^4 - 132x^3 - 417x^2 + 103x + 8)\mu_5 \\ & + (1176x^5 - 264x^4 - 1128x^3 + 272x^2 + 146x - 22)\mu_6 \geq 0 \end{aligned}$$

and

$$\begin{aligned} p(x) = & 1 - x\mu_1 - (2x^2 - 1)\mu_2 - (4x^3 - 3x)\mu_3 - (8x^4 - 8x^2 + 1)\mu_4 \\ & - (16x^5 - 20x^3 + 5x)\mu_5 - (32x^6 - 48x^4 + 18x^2 - 1)\mu_6 > 0, \end{aligned}$$

respectively, for all $x \in [-1, 1]$. In Table 2.1, we list several multipliers satisfying these conditions.

Furthermore, evaluating P at $x = 3/40$, we have

$$P\left(\frac{3}{40}\right) < -15.1563 + 13.7341 \sum_{i=1}^6 |\mu_i|.$$

Assuming $|\mu_1| + \dots + |\mu_6| \leq 1$, we observe that

$$P\left(\frac{3}{40}\right) < -1.4222 < 0,$$

and infer that no Nevanlinna–Odeh multiplier exists for the six-step BDF method.

Table 2.1

Multipliers for the six-step BDF method; see also (2.4).

μ_1	μ_2	μ_3	μ_4	μ_5	μ_6
1.6	-0.92	0.3	0	0	0
0.8235	-0.855	0.38	0	0	0
1.67	-1	0.4	-0.1	0	0
0.8	-0.7	0.2	0.1	0	0
1.118	-1	0.6	-0.2	0.2	0
0.6708	-0.2	-0.2	0.6	-0.2	0
0.735	-0.2	-0.4	0.8	-0.4	0.2

3. Stability. In this section we establish two stability estimates for the six-step BDF method (1.3) by the energy technique which are discrete analogues of the standard stability estimates for the continuous problem (1.1) that are obtained by the energy technique when testing by u and u' , respectively; namely

$$(3.1) \quad |u(t)|^2 + \int_0^t \|u(s)\|^2 ds \leq |u^0|^2 + \int_0^t \|f(s)\|_*^2 ds, \quad 0 < t \leq T,$$

and

$$(3.2) \quad \|u(t)\|^2 + \int_0^t |u'(s)|^2 ds \leq \|u^0\|^2 + \int_0^t |f(s)|^2 ds, \quad 0 < t \leq T.$$

The second stability result for the six-step BDF method is new, while the first is well known; the novelty in the first case lies in the simplicity of the proof. The analogue of the second stability estimate played a key role in the analysis of fully discrete methods for mean curvature flow of closed surfaces in [17] and for the Landau–Lifshitz–Gilbert equation in [3], where linearly implicit variants of BDF methods up to order 5 are used for the discretization in time. Proofs of the first stability estimate for the six-step BDF method by other stability techniques are significantly more involved. For a proof by a spectral technique in the case of selfadjoint operators, we refer to [24, chapter 10]; for a proof in the general case, under a sharp condition on the nonselfadjointness of the operator as well as for nonlinear parabolic equations, by a combination of spectral and Fourier techniques, see, e.g., [2] and references therein. For a long-time estimate in the case of selfadjoint operators and an application to the Stokes–Darcy problem, see [18]. We also extend the first stability estimate to the case of nonautonomous equations.

For simplicity, we denote by $\langle \cdot, \cdot \rangle$ the inner product on V , $\langle v, w \rangle := (A^{1/2}v, A^{1/2}w)$.

Before we proceed, for the reader's convenience, we recall the notion of the generating function of an $n \times n$ Toeplitz matrix T_n as well as an auxiliary result, the Grenander–Szegő theorem, which plays a key role in our analysis.

Definition 3.1 ([10, p. 13]; the generating function of a Toeplitz matrix). Consider the $n \times n$ Toeplitz matrix

$$T_n = (t_{ij})_{i,j=1,\dots,n} \in \mathbb{C}^{n,n}$$

with diagonal entries t_0 , subdiagonal entries t_1 , superdiagonal entries t_{-1} , and so on, and $(n, 1)$ and $(1, n)$ entries t_{n-1} and t_{1-n} , respectively, i.e., the entries $t_{ij} = t_{i-j}$, $i, j = 1, \dots, n$, are constant along the diagonals of T_n . Let t_{-n+1}, \dots, t_{n-1} be the Fourier coefficients of the trigonometric polynomial g of degree less than or equal to $n-1$, i.e.,

$$t_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(x) e^{-ikx} dx, \quad k = 1-n, \dots, n-1.$$

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

If the generating function g is real-valued, then the matrix T_n is Hermitian; if g is real-valued and even, then T_n is symmetric.

Lemma 3.2 ([10, pp. 13–14]; the Grenander–Szegő theorem). *Let T_n be a symmetric Toeplitz matrix as in Definition 3.1 with generating function g . Then, the smallest and largest eigenvalues $\lambda_{\min}(T_n)$ and $\lambda_{\max}(T_n)$, respectively, of T_n are bounded as follows*

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

with g_{\min} and g_{\max} the minimum and maximum of g , respectively. In particular, if g_{\min} is positive, then the symmetric matrix T_n is positive definite.¹

Notice, in particular, that the generating function of a *symmetric* band Toeplitz matrix T_n of bandwidth $2m + 1$, i.e., with $t_{m+1} = \dots = t_{n-1} = 0$, is a real-valued, even trigonometric polynomial of degree m , $g(x) = t_0 + 2t_1 \cos x + \dots + 2t_m \cos(mx)$, for all $n \geq m + 1$.

In the proofs of the stability Theorems 3.3 and 3.6, we shall use the fact that the positive function g of (2.12) is the generating function of seven-diagonal, $m = 3$, symmetric Toeplitz matrices; according to the Grenander–Szegő theorem, these matrices are positive definite; this is the point where the positivity property (P2) for the multiplier (2.4) of the six-step BDF method will play a crucial role.

3.1. First stability estimate. Here we establish a discrete analogue of the stability estimate (3.1) for the six-step BDF method by the energy technique.

Theorem 3.3 (Stability of the six-step BDF method). *Let $u^0, u^1, \dots, u^5 \in V$. The six-step BDF method (1.3) is stable in the sense that*

$$(3.3) \quad |u^n|^2 + \tau \sum_{\ell=6}^n \|u^\ell\|^2 \leq C \sum_{j=0}^5 (|u^j|^2 + \tau \|u^j\|^2) + C\tau \sum_{\ell=6}^n \|f^\ell\|_*^2, \quad n = 6, \dots, N.$$

Here C denotes a generic constant depending only on the numerical method, i.e., independent of T and the operator A as well as of f, τ and n .

Proof. Taking in (1.3) the inner product with $u^{n+6} - \frac{13}{9}u^{n+5} + \frac{25}{36}u^{n+4} - \frac{1}{9}u^{n+3}$, cf. (2.2) and (2.4), we have

$$(3.4) \quad \left(\sum_{i=0}^6 \alpha_i u^{n+i}, u^{n+6} - \sum_{j=1}^3 \mu_j u^{n+6-j} \right) + \tau A_{n+6} = \tau F_{n+6}$$

with

$$A_{n+6} := \left\langle u^{n+6}, u^{n+6} - \sum_{j=1}^3 \mu_j u^{n+6-j} \right\rangle \quad \text{and} \quad F_{n+6} := \left(f^{n+6}, u^{n+6} - \sum_{j=1}^3 \mu_j u^{n+6-j} \right);$$

cf. (2.3).

With the notation $\mathcal{U}^n := (u^{n-5}, u^{n-4}, u^{n-3}, u^{n-2}, u^{n-1}, u^n)^\top$ and the norm $|\mathcal{U}^n|_G$ given by

$$|\mathcal{U}^n|_G^2 = \sum_{i,j=1}^6 g_{ij} (u^{n-6+i}, u^{n-6+j}),$$

using (G), we have

$$(3.5) \quad \left(\sum_{i=0}^6 \alpha_i u^{n+i}, u^{n+6} - \sum_{j=1}^3 \mu_j u^{n+6-j} \right) \geq |\mathcal{U}^{n+6}|_G^2 - |\mathcal{U}^{n+5}|_G^2.$$

¹For real-valued g and $z = (z_0, \dots, z_{n-1})^\top \in \mathbb{C}^n$, we have $(T_n z, z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} g(x) \left| \sum_{k=0}^{n-1} z_k e^{ikx} \right|^2 dx$ and $(z, z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left| \sum_{k=0}^{n-1} z_k e^{ikx} \right|^2 dx$, and the result is evident.

Thus, (3.4) yields

$$(3.6) \quad |\mathcal{U}^{n+6}|_G^2 - |\mathcal{U}^{n+5}|_G^2 + \tau A_{n+6} \leq \tau F_{n+6}.$$

Summing in (3.6) from $n = 0$ to $n = m - 6$, we obtain

$$(3.7) \quad |\mathcal{U}^m|_G^2 - |\mathcal{U}^5|_G^2 + \tau \sum_{n=6}^m A_n \leq \tau \sum_{n=6}^m F_n.$$

The sum on the right-hand side can be easily estimated by the generalized Cauchy–Schwarz inequality and the arithmetic–geometric mean inequality with a suitable weight. We next focus on the estimation of the sum $A_6 + \dots + A_m$ from below; we have

$$(3.8) \quad \sum_{n=6}^m A_n = \sum_{n=6}^m \left\langle u^n, u^n - \sum_{j=1}^3 \mu_j u^{n-j} \right\rangle.$$

First, motivated by the positivity of the function g of (2.12), to take advantage of the positivity property (P2), we introduce the notation $\mu_0 := -31/32$, and rewrite (3.8) as

$$(3.9) \quad \sum_{n=6}^m A_n = \frac{1}{32} \sum_{n=6}^m \|u^n\|^2 + J_m \quad \text{with} \quad J_m := - \sum_{j=0}^3 \mu_j \sum_{i=1}^{m-5} \langle u^{5+i}, u^{5+i-j} \rangle.$$

Our next task is to rewrite J_m in a form that will enable us to estimate it from below in a desired way. To this end, we introduce the lower triangular Toeplitz matrix $L = (\ell_{ij}) \in \mathbb{R}^{m-5, m-5}$ with entries

$$\ell_{i, i-j} = -\mu_j, \quad j = 0, 1, 2, 3, \quad i = j + 1, \dots, m - 5,$$

and all other entries equal zero. With this notation, we have

$$\sum_{i, j=1}^{m-5} \ell_{ij} \langle u^{5+i}, u^{5+j} \rangle = - \sum_{j=0}^3 \mu_j \sum_{i=j+1}^{m-5} \langle u^{5+i}, u^{5+i-j} \rangle,$$

i.e.,

$$(3.10) \quad \sum_{i, j=1}^{m-5} \ell_{ij} \langle u^{5+i}, u^{5+j} \rangle = J_m + \langle u^6, \mu_1 u^5 + \mu_2 u^4 + \mu_3 u^3 \rangle \\ + \langle u^7, \mu_2 u^5 + \mu_3 u^4 \rangle + \langle u^8, \mu_3 u^5 \rangle.$$

At this point we shall use the positivity property (P2) to show that the term on the left-hand side of (3.10) is nonnegative and then obtain a suitable lower bound for J_m . Indeed, the symmetric part

$$L_s := (L + L^\top)/2$$

of the matrix L is a symmetric seven-diagonal Toeplitz matrix and its generating function g , see (2.12), is positive. Hence, according to the Grenander–Szegő theorem, see Lemma 3.2, the Toeplitz matrix L_s is positive definite. Consequently, since

$$(Lx, x) = (L_s x, x) \quad \forall x \in \mathbb{R}^{m-5},$$

the matrix L is also positive definite. Therefore, the expression on the left-hand side of (3.10) is nonnegative; thus, (3.10) yields the desired estimate for J_m from below, i.e.,

$$(3.11) \quad J_m \geq -\langle u^6, \mu_1 u^5 + \mu_2 u^4 + \mu_3 u^3 \rangle - \langle u^7, \mu_2 u^5 + \mu_3 u^4 \rangle - \langle u^8, \mu_3 u^5 \rangle.$$

From (3.7), (3.9) and (3.11), we obtain

$$(3.12) \quad |\mathcal{U}^m|_G^2 + \frac{1}{32} \tau \sum_{n=6}^m \|u^n\|^2 \leq |\mathcal{U}^5|_G^2 + \tau \sum_{n=6}^m F_n + \tau \langle u^6, \mu_1 u^5 + \mu_2 u^4 + \mu_3 u^3 \rangle \\ + \tau \langle u^7, \mu_2 u^5 + \mu_3 u^4 \rangle + \tau \langle u^8, \mu_3 u^5 \rangle.$$

Now, with c_1 and c_2 the smallest and largest eigenvalues of the matrix G , we have

$$(3.13) \quad |\mathcal{U}^m|_G^2 \geq c_1 |u^m|^2 \quad \text{and} \quad |\mathcal{U}^5|_G^2 \leq c_2 \sum_{j=0}^5 |u^j|^2.$$

Furthermore, the terms involving the forcing term or the starting approximations can be estimated by elementary inequalities in the form

$$(3.14) \quad F_n \leq \frac{1}{4\varepsilon_1} \left(1 + \sum_{j=1}^3 |\mu_j|\right) \|f^n\|_*^2 + \varepsilon_1 \left(\|u^n\|^2 + \sum_{j=1}^3 |\mu_j| \|u^{n-j}\|^2\right)$$

and

$$(3.15) \quad |\langle u^i, u^j \rangle| \leq \varepsilon_2 \|u^i\|^2 + \frac{1}{4\varepsilon_2} \|u^j\|^2, \quad i = 6, 7, 8, \quad j = 3, 4, 5,$$

with sufficiently small ε_1 and ε_2 . Inserting (3.13), (3.14), and (3.15) into (3.12), we easily obtain the desired stability estimate (3.3). ■

Remark 3.4. Let us also note that, due to the fact that $\mu_4 = \mu_5 = \mu_6 = 0$, the terms $\|u^2\|^2$, $\|u^1\|^2$ and $\|u^0\|^2$ are actually not needed on the right-hand side of (3.3). In other words, it suffices to assume that $u^0, u^1, u^2 \in H$ and $u^3, u^4, u^5 \in V$.

Proposition 3.5 (Error estimate). *Assume that the solution u of (1.1) is sufficiently smooth and that the starting approximations $u^0, u^1, \dots, u^5 \in V$ to $u(t^0), \dots, u(t^5)$ are such that*

$$(3.16) \quad \max_{0 \leq j \leq 5} \left(|u(t^j) - u^j| + \tau^{1/2} \|u(t^j) - u^j\| \right) \leq C\tau^6.$$

Then, we have the error estimate

$$(3.17) \quad \max_{0 \leq n \leq N} |u(t^n) - u^n| \leq C\tau^6$$

with a constant C independent of τ .

Proof. Let d^ℓ denote the consistency error of the six-step BDF method (1.3) (with $q = 6$) for the initial value problem (1.1), i.e., the amount by which the exact solution u of (1.1) misses satisfying the numerical method,

$$(3.18) \quad \tau d^{n+6} = \sum_{i=0}^6 \alpha_i u(t^{n+i}) + \tau A u(t^{n+6}) - \tau f^{n+6}, \quad n = 0, \dots, N-6.$$

In view of the differential equation in (1.1), we can write (3.18) in the form

$$\tau d^{n+6} = \sum_{i=0}^6 \alpha_i u(t^{n+i}) - \tau u'(t^{n+6}), \quad n = 0, \dots, N-6.$$

The order of the six-step method is 6, i.e.,

$$(3.19) \quad \sum_{i=0}^q i^\ell \alpha_i = \ell 6^{\ell-1}, \quad \ell = 0, 1, \dots, 6.$$

Now, by Taylor expanding about t^n and using the order conditions (3.19), we obtain

$$\tau d^{n+6} = \frac{1}{6!} \left[\sum_{i=0}^6 \alpha_i \int_{t^n}^{t^{n+i}} (t^{n+i} - s)^6 u^{(7)}(s) ds - 6\tau \int_{t^n}^{t^{n+6}} (t^{n+6} - s)^5 u^{(7)}(s) ds \right]$$

$n = 0, \dots, N-6$. Thus, under obvious regularity requirements, we obtain the desired optimal order consistency estimate

$$(3.20) \quad \max_{6 \leq \ell \leq N} \|d^\ell\|_* \leq C\tau^6.$$

Subtracting the six-step BDF method (1.3) from (3.18), we obtain the error equation

$$(3.21) \quad \sum_{i=0}^6 \alpha_i e^{n+i} + \tau A e^{n+q} = \tau d^{n+q}, \quad n = 0, \dots, N-6,$$

for the error $e^\ell := u(t^\ell) - u^\ell$, $\ell = 0, \dots, N$.

The stability estimate (3.3) for the error equation (3.21) in combination with the consistency estimate (3.20) and our assumption (3.16) on the starting approximations leads to the claimed error estimate (3.17). ■

3.2. Second stability estimate. Here we establish a discrete analogue of the stability estimate (3.2) for the six-step BDF method by the energy technique. Stability estimates of this form for BDF methods of order up to 5 are derived in [17, 3] via Nevanlinna–Odeh multipliers; these estimates played a key role in the analyses in [17, 3].

For simplicity of notation, we indicate by a dot the application of the six-step backward difference operator to a sequence v^0, \dots, v^N ,

$$(3.22) \quad \dot{v}^{n+6} := \frac{1}{\tau} \sum_{i=0}^6 \alpha_i v^{n+i}, \quad n = 0, \dots, N-6,$$

and write the six-step BDF method (1.3), with $q = 6$, in the form

$$(3.23) \quad \dot{u}^n + Au^n = f^n, \quad n = 6, \dots, N.$$

Theorem 3.6 (Stability of the six-step BDF method). *Let $u^0, u^1, \dots, u^5 \in V$. The six-step BDF method (3.23) is stable in the sense that*

$$(3.24) \quad \|u^n\|^2 + \tau \sum_{\ell=6}^n |\dot{u}^\ell|^2 \leq C \sum_{j=0}^5 \|u^j\|^2 + C\tau \sum_{\ell=6}^n |f^\ell|^2, \quad n = 6, \dots, N.$$

Here C denotes a generic constant depending only on the numerical method, i.e., independent of T and the operator A as well as of f, τ and n .

Proof. For $n \geq 9$, to take advantage of the properties of the multiplier (2.4), we consider method (3.23) with n replaced by $n-j$, multiply it by $\mu_j, j = 1, 2, 3$, and subtract the resulting relations from (3.23), to obtain

$$(3.25) \quad \dot{u}^n - \sum_{j=1}^3 \mu_j \dot{u}^{n-j} + A \left(u^n - \sum_{j=1}^3 \mu_j u^{n-j} \right) = f^n - \sum_{j=1}^3 \mu_j f^{n-j}, \quad n = 9, \dots, N.$$

Taking in (3.25) the inner product with \dot{u}^n , we obtain

$$(3.26) \quad I_n + \left\langle \dot{u}^n, u^n - \sum_{j=1}^3 \mu_j u^{n-j} \right\rangle = \tilde{F}_n, \quad n = 9, \dots, N,$$

with

$$I_n := \left(\dot{u}^n, \dot{u}^n - \sum_{j=1}^3 \mu_j \dot{u}^{n-j} \right) \quad \text{and} \quad \tilde{F}_n := \left(f^n - \sum_{j=1}^3 \mu_j f^{n-j}, \dot{u}^n \right).$$

With the notation $\mathcal{U}^n := (u^{n-5}, u^{n-4}, u^{n-3}, u^{n-2}, u^{n-1}, u^n)^\top$ and the norm $\|\mathcal{U}^n\|_G$ given by

$$\|\mathcal{U}^n\|_G^2 = \sum_{i,j=1}^6 g_{ij} \langle u^{n-6+i}, u^{n-6+j} \rangle,$$

using (G), in view of (3.22), we have

$$\tau \left\langle \dot{u}^n, u^n - \sum_{j=1}^3 \mu_j u^{n-j} \right\rangle \geq \|\mathcal{U}^n\|_G^2 - \|\mathcal{U}^{n-1}\|_G^2;$$

cf. (3.5).

Therefore, (3.26) yields

$$(3.27) \quad \|\mathcal{U}^n\|_G^2 - \|\mathcal{U}^{n-1}\|_G^2 + \tau I_n \leq \tau \tilde{F}_n.$$

Summing up in (3.27) from $n = 9$ to $n = m \leq N$, we obtain

$$\|\mathcal{U}^m\|_G^2 - \|\mathcal{U}^8\|_G^2 + \tau \sum_{n=9}^m I_n \leq \tau \sum_{n=9}^m \tilde{F}_n.$$

Proceeding as in the proof of Theorem 3.3, we arrive at the estimate

$$(3.28) \quad \begin{aligned} \|\mathcal{U}^m\|_G^2 + \frac{1}{32} \tau \sum_{n=9}^m |\dot{u}^n|^2 &\leq \|\mathcal{U}^8\|_G^2 + \tau \sum_{n=9}^m \tilde{F}_n + \tau (\dot{u}^9, \mu_1 \dot{u}^8 + \mu_2 \dot{u}^7 + \mu_3 \dot{u}^6) \\ &\quad + \tau (\dot{u}^{10}, \mu_2 \dot{u}^8 + \mu_3 \dot{u}^7) + \tau (\dot{u}^{11}, \mu_3 \dot{u}^8), \end{aligned}$$

$m = 9, \dots, N$. Notice that the differences in the upper indices in the last three terms on the right-hand sides of (3.12) and (3.28) are due to the fact that the summation in (3.12) and (3.28) starts at $n = 6$ and $n = 9$, respectively.

Now, with c_1 and c_2 the smallest and largest eigenvalues of the matrix G , we have

$$(3.29) \quad \|U^m\|_G^2 \geq c_1 \|u^m\|^2 \quad \text{and} \quad \|U^8\|_G^2 \leq c_2 \sum_{j=3}^8 \|u^j\|^2.$$

Furthermore, the terms involving the forcing term or the starting approximations can be estimated by elementary inequalities in the form

$$(3.30) \quad \tilde{F}_n \leq \frac{1}{4\varepsilon_1} \left(|f^n|^2 + \sum_{j=1}^3 |\mu_j| |f^{n-j}|^2 \right) + \varepsilon_1 \left(1 + \sum_{j=1}^3 |\mu_j| \right) |\dot{u}^n|^2$$

and

$$(3.31) \quad |(\dot{u}^i, \dot{u}^j)| \leq \varepsilon_2 |\dot{u}^i|^2 + \frac{1}{4\varepsilon_2} |\dot{u}^j|^2, \quad i = 9, 10, 11, \quad j = 6, 7, 8,$$

with sufficiently small ε_1 and ε_2 . Inserting (3.29), (3.30), and (3.31) into (3.28), we easily obtain

$$\|u^m\|^2 + \tau \sum_{\ell=6}^m |\dot{u}^\ell|^2 \leq C \sum_{j=3}^8 \|u^j\|^2 + C\tau \sum_{j=6}^8 |\dot{u}^j|^2 + C\tau \sum_{\ell=6}^m |f^\ell|^2, \quad m = 9, \dots, N.$$

To complete the proof of the desired stability estimate (3.24), it remains to show that

$$(3.32) \quad \|u^m\|^2 + \tau |\dot{u}^m|^2 \leq c \sum_{j=0}^5 \|u^j\|^2 + c\tau \sum_{\ell=6}^m |f^\ell|^2, \quad m = 6, 7, 8.$$

This can be done via elementary inequalities; cf. [3, Appendix]. Testing (3.23) for $n = 6$ by \dot{u}^6 , we have

$$|\dot{u}^6|^2 + \frac{\alpha_6}{\tau} \|u^6\|^2 = -\frac{1}{\tau} \sum_{i=0}^5 \alpha_i \langle u^6, u^i \rangle + (f^6, \dot{u}^6).$$

Estimating the terms on the right-hand side in the form $|\langle u^6, u^i \rangle| \leq \varepsilon' \|u^6\|^2 + \|u^i\|^2 / (4\varepsilon')$ with sufficiently small ε' and $2(f^6, \dot{u}^6) \leq |f^6|^2 + |\dot{u}^6|^2$, we easily obtain (3.32) for $m = 6$. Then, using (3.32) for $m = 6$, we similarly obtain the desired result for $m = 7$, and subsequently also for $m = 8$. ■

Remark 3.7 (Error estimate). The stability estimate (3.24) applied to the error equation (3.21), in combination with the analogue of the consistency estimate (3.20) in the H -norm $|\cdot|$, leads to the optimal order error estimate

$$\max_{6 \leq n \leq N} \|u(t^n) - u^n\| \leq C\tau^6$$

with a constant C independent of τ , provided that the errors of the starting values u^0, \dots, u^5 also satisfy such an estimate; cf. Proposition 3.5.

3.3. Nonautonomous equations. In this section we use the stability result of Theorem 3.3 to establish stability of the six-step BDF method for nonautonomous equations.

We consider the initial value problem, for simplicity for a homogeneous equation,

$$(3.33) \quad \begin{cases} u'(t) + A(t)u(t) = 0, & 0 < t < T, \\ u(0) = u^0, \end{cases}$$

with positive definite selfadjoint operators $A(t) : V \rightarrow V', t \in [0, T]$.

For concreteness, we define the norm on V in terms of $A(0)$, i.e., $\|v\| := |A(0)^{1/2}v|$. Our structural assumptions are that all operators $A(t), t \in [0, T]$, share the same domain, produce equivalent norms on V ,

$$(3.34) \quad |A(t)^{1/2}v| \leq c|A(\tilde{t})^{1/2}v| \quad \forall t, \tilde{t} \in [0, T] \quad \forall v \in V,$$

and $A(t) : V \rightarrow V'$ is of bounded variation with respect to t ,

$$(3.35) \quad |A(s)^{-1/2}(A(t) - A(\tilde{t}))v| \leq [\sigma(t) - \sigma(\tilde{t})]|A(s)^{1/2}v|, \quad 0 \leq \tilde{t} \leq t \leq T, \quad \forall v \in V,$$

for every $s \in [0, T]$, with an increasing function $\sigma : [0, T] \rightarrow \mathbb{R}$.

Clearly, $c \geq 1$ in (3.34), and the analogue of (3.34) holds true also for the dual norms $|A(t)^{-1/2} \cdot |$ with the same constant c . Let us also note that (3.35) takes the form

$$\|(A(t) - A(\tilde{t}))v\|_* \leq [\sigma(t) - \sigma(\tilde{t})]\|v\|, \quad 0 \leq \tilde{t} \leq t \leq T, \quad \forall v \in V,$$

for $s = 0$. Furthermore, if (3.35) is valid for a fixed $s \in [0, T]$, then, in view of (3.34), it is valid for any $s \in [0, T]$ with the right-hand side, that is with σ , multiplied by c^2 .

Now, the six-step BDF method for the initial value problem (3.33) is

$$(3.36) \quad \sum_{i=0}^6 \alpha_i u^{n+i} + \tau A(t^{n+6})u^{n+6} = 0, \quad n = 0, \dots, N-6,$$

assuming that starting approximations $u^0, \dots, u^5 \in V$ are given. The next theorem provides a stability estimate of the scheme (3.36).

Theorem 3.8 (Stability of the six-step BDF method for nonautonomous equations). *Let $u^0, u^1, \dots, u^5 \in V$. Assume that the time-dependent, positive definite selfadjoint operators $A(t) : V \rightarrow V', t \in [0, T]$, satisfy the conditions (3.34) and (3.35). Then, the six-step BDF method (3.36) is stable in the sense that*

$$(3.37) \quad |u^n|^2 + \tau \sum_{\ell=6}^n \|u^\ell\|^2 \leq \tilde{C} \sum_{j=0}^5 (|u^j|^2 + \tau \|u^j\|^2), \quad n = 6, \dots, N.$$

Here, \tilde{C} is a constant independent of $s, A(t), \tau$ and n that depends exponentially on T .

Proof. Let us fix an $6 \leq m \leq N$. From (3.36), we obtain

$$\sum_{i=0}^6 \alpha_i u^{n+i} + \tau A(t^m)u^{n+6} = \tau [A(t^m) - A(t^{n+6})]u^{n+6}, \quad n = 0, \dots, m-6.$$

Since the time t is frozen at t^m in the operator $A(t^m)$ on the left-hand side, we can apply the already-established stability estimate (3.3), for the time-independent operator $A := A(t^m)$, with perturbation terms $f^\ell := [A(t^m) - A(t^\ell)]u^\ell$ and obtain

$$(3.38) \quad |u^m|^2 + \tau \sum_{\ell=6}^m |A(t^m)^{1/2}u^\ell|^2 \leq C \sum_{j=0}^5 (|u^j|^2 + \tau |A(t^m)^{1/2}u^j|^2) + CM^m$$

with a constant C independent of τ and m , and

$$M^m := \tau \sum_{\ell=6}^m |A(t^m)^{-1/2}[A(t^m) - A(t^\ell)]u^\ell|^2.$$

Using (3.34) and its analogue for the dual norms, we infer from (3.38) that

$$(3.39) \quad |u^m|^2 + \tau \sum_{\ell=6}^m \|u^\ell\|^2 \leq C_1 \sum_{j=0}^5 (|u^j|^2 + \tau \|u^j\|^2) + C_1 M^m$$

with the constant $C_1 := c^4 C$. Now, with

$$E^\ell := \tau \sum_{j=6}^{\ell} \|u^j\|^2, \quad \ell = 6, \dots, m, \quad E^5 := 0,$$

estimate (3.39) yields

$$(3.40) \quad E^m \leq C_1 \sum_{j=0}^5 (|u^j|^2 + \tau \|u^j\|^2) + C_1 M^m.$$

Furthermore, in view of the bounded variation condition (3.35),

$$M^m \leq \tau \sum_{\ell=6}^{m-1} [\sigma(t^m) - \sigma(t^\ell)]^2 \|u^\ell\|^2 = \sum_{\ell=6}^{m-1} [\sigma(t^m) - \sigma(t^\ell)]^2 (E^\ell - E^{\ell-1}),$$

whence, by summation by parts, we have

$$(3.41) \quad M^m \leq \sum_{\ell=6}^{m-1} a_\ell E^\ell,$$

with $a_\ell := [\sigma(t^m) - \sigma(t^\ell)]^2 - [\sigma(t^m) - \sigma(t^{\ell+1})]^2 \geq 0$, and (3.40) yields

$$(3.42) \quad E^m \leq C_1 \sum_{j=0}^5 (|u^j|^2 + \tau \|u^j\|^2) + C_1 \sum_{\ell=6}^{m-1} a_\ell E^\ell.$$

Note that the sum $\sum_{\ell=6}^{m-1} a_\ell$ is uniformly bounded by a constant independent of m and the time step τ ,

$$\sum_{\ell=6}^{m-1} a_\ell = [\sigma(t^m) - \sigma(t^6)]^2 \leq [\sigma(T) - \sigma(0)]^2.$$

Therefore, a discrete Gronwall-type argument applied to (3.42) leads to

$$(3.43) \quad E^m \leq C_2 \sum_{j=0}^5 (|u^j|^2 + \tau \|u^j\|^2).$$

Combining (3.39) with (3.41) and (3.43), we obtain the desired stability estimate (3.37) for the case of nonautonomous equations. \blacksquare

4. Numerical results. We applied three time-stepping methods, the six-step BDF method and two popular Runge–Kutta methods, namely the three-stage (fifth order) Radau IIA and (sixth order) Gauss methods to initial and boundary value problems for the equation

$$(4.1) \quad u_t - \Delta u + u = f \quad \text{in } \Omega \times [0, T],$$

with $\Omega = (-1, 1)^2$ and $T = 1$, subject to *periodic* and to *Dirichlet* boundary conditions, respectively. In both cases, in space we discretized by the spectral collocation method with the Chebyshev–Gauss–Lobatto points.

For the reader's convenience, we present the Butcher tableaus of the three-stage Radau IIA and Gauss methods, respectively,

$$(4.2) \quad \begin{array}{ccc|c} \frac{88-7\sqrt{6}}{360} & \frac{296-169\sqrt{6}}{1800} & \frac{-2+3\sqrt{6}}{225} & \frac{4-\sqrt{6}}{10} \\ \frac{296+169\sqrt{6}}{1800} & \frac{88+7\sqrt{6}}{360} & \frac{-2-3\sqrt{6}}{225} & \frac{4+\sqrt{6}}{10} \\ \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} & 1 \\ \hline \frac{16-\sqrt{6}}{36} & \frac{16+\sqrt{6}}{36} & \frac{1}{9} & \end{array} =: \frac{\mathcal{Q}}{b^\top} \Big| c$$

and

$$(4.3) \quad \begin{array}{ccc|c} \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} & \frac{1}{2} - \frac{\sqrt{15}}{10} \\ \frac{5}{36} + \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} & \frac{1}{2} \\ \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} & \frac{1}{2} + \frac{\sqrt{15}}{10} \\ \hline \frac{5}{18} & \frac{4}{9} & \frac{5}{18} & \end{array} =: \frac{\mathcal{Q}}{b^\top} \Big| c.$$

Let us also briefly recall some well-known facts about Radau IIA and Gauss methods; for details we refer to [13]. Both classes of methods are of collocation type, i.e., the *stage order* of their q -stage members is q . The *order* p of the q -stage Radau IIA and Gauss methods is $p = 2q - 1$ and $p = 2q$, respectively, the weights b_1, \dots, b_q are positive, and the $q \times q$ symmetric matrices M with entries $m_{ij} := b_i a_{ij} + b_j a_{ji} - b_i b_j$, $i, j = 1, \dots, q$, are positive semidefinite; actually, in the case of the Gauss methods, $M = 0$. In particular, the methods are *algebraically stable*, whence also A- and B-stable. The stability functions r ,

$$r(z) := 1 + z b^\top (I - z \mathcal{Q})^{-1} \mathbb{1} \quad \text{with } \mathbb{1} := (1, \dots, 1)^\top \in \mathbb{R}^q,$$

vanish at infinity in the case of the Radau IIA methods, $r(\infty) = 1 - b^\top \mathcal{Q}^{-1} \mathbb{1} = 0$, whence these methods are *strongly A-stable*, while in the case of the q -stage Gauss method, we have $r(\infty) = (-1)^q$. The first members of the Radau IIA and Gauss families, respectively, for $q = 1$, are the implicit Euler and the implicit midpoint (or Crank–Nicolson) methods. Note that the

computational cost of implicit Runge–Kutta methods increases fast with the stage number; we refer to [9, 15, 14] and the reference therein for efficient implementations.

We numerically verified the theoretical results including convergence orders in the discrete L^2 -norm. We express the space discrete approximation u_I^n in terms of its values at Chebyshev–Gauss–Lobatto points,

$$u_I^n(x, y) = \sum_{i=0}^{N_x} \sum_{j=0}^{N_y} u_{ij}^n \ell_i(x) \ell_j(y), \quad \ell_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{N_x} \frac{x - x_j}{x_i - x_j},$$

where $u_{ij}^n := u_I^n(x_i, y_j)$ at the mesh points (x_i, y_j) . Here, $-1 = x_0 < x_1 < \dots < x_{N_x} = 1$ and $-1 = y_0 < y_1 < \dots < y_{N_y} = 1$ are nodes of Lobatto quadrature rules for the weight function $w(x) = 1/(1 - x^2)^{1/2}$. In order to test the temporal error, we fix $N_x = N_y = 20$; the spatial error is negligible since the spectral collocation method converges exponentially; see, e.g., [23, Theorem 4.4, §4.5.2].

Example 4.1 (Periodic boundary conditions). Here, the initial value and the forcing term were chosen such that the exact solution of equation (4.1) is

$$(4.4) \quad u(x, y, t) = (t^7 + 1) \sin(\pi x) \sin(\pi y), \quad -1 \leq x, y \leq 1, \quad 0 \leq t \leq 1.$$

For this case, we present in Table 4.1 the L^2 -norm of the errors as well as the corresponding convergence orders (rates) for the six-step BDF (BDF6) scheme and for the three-stage Gauss and Radau IIA methods.

Table 4.1

Example 4.1: The discrete L^2 -norm errors and numerical convergence orders with $N_x = N_y = 20$.

τ	BDF6	Rate	Gauss	Rate	Radau IIA	Rate
1/30	5.8572e-08		7.8948e-09		1.5660e-07	
1/60	9.1075e-10	6.0070	1.2465e-10	5.9849	5.0927e-09	4.9425
1/90	8.0012e-11	5.9983	1.0966e-11	5.9948	6.7881e-10	4.9702
1/120	1.4235e-11	6.0014	1.9549e-12	5.9945	1.6202e-10	4.9798

Example 4.2 (Dirichlet boundary conditions). Here, the initial value, the nonhomogeneous Dirichlet boundary conditions, and the forcing term were chosen such that the exact solution of equation (4.1) is

$$(4.5) \quad u(x, y, t) = (t^7 + 1) \sin(x) \sin(\pi y), \quad -1 \leq x, y \leq 1, \quad 0 \leq t \leq 1.$$

Notice that u is not periodic in x .

For the solution u given in (4.5), we present in Table 4.2 the L^2 -norm of the errors as well as the corresponding convergence orders for the six-step BDF scheme and for the three-stage Gauss and Radau IIA methods. Notice the order reduction, due to the lack of restrictive compatibility conditions, in the cases of the three-stage Gauss and Radau IIA methods; although the solution is very smooth, the computational order is slightly higher than 4 (i.e., $q + 1$), rather than the classical orders 6 and 5, respectively, of these methods. See [24, chapter 8] and references therein. In the case of periodic boundary conditions, smooth solutions satisfy the required compatibility conditions and no order reduction occurs. In contrast to

Table 4.2

Example 4.2: The discrete L^2 -norm errors and numerical convergence orders with $N_x = N_y = 20$.

τ	BDF6	Rate	Gauss	Rate	Radau IIA	Rate
1/30	3.7026e-08		5.7181e-07		3.2137e-07	
1/60	5.7732e-10	6.0030	3.1237e-08	4.1942	1.7868e-08	4.1688
1/90	5.0674e-11	6.0005	5.6615e-09	4.2123	3.3155e-09	4.1542
1/120	9.0168e-12	6.0008	1.6781e-09	4.2270	1.0053e-09	4.1479

Runge–Kutta methods, multistep methods do not suffer from order reduction because their consistency errors can be expressed in terms of the solution u only; neither the elliptic operator nor the forcing terms enter into their consistency errors. Of course, implicit Runge–Kutta methods are superior to multistep methods for certain classes of parabolic equations as they can combine excellent stability properties, such as A- or B-stability, with arbitrarily high order of accuracy.

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