THE ENERGY TECHNIQUE FOR THE SIX-STEP BDF METHOD

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1. Supplement

This is a supplement to the slides of the talk entitled "The energy technique for the six-step BDF method", I gave in the Irish Numerical Analysis Forum (INAF) seminar series on January 13, 2022. Its scope is to provide details and references to the literature of the answers I gave to interesting questions of two of the organizers of INAF, namely, Natalia Kopteva and Martin Stynes.

Let $T > 0$ and $u^0 \in H$, and consider the initial value problem, for a linear abstract parabolic equation,

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

in a usual triple of separable complex Hilbert spaces $V \subset H = H' \subset V'$, with V densely and continuously embedded in H. We assume that (1.1) possesses a unique, smooth solution.

Let (α, β) be an implicit q-step method, generated by two polynomials α and β, of degree q,

$$\alpha(\zeta) = \sum_{i=0}^{q} \alpha_i \zeta^i, \quad \beta(\zeta) = \sum_{i=0}^{q} \beta_i \zeta^i,$$

with real coefficients α_i and β_i.

Let $N \in \mathbb{N}, \tau := T/N$ be the constant time step, and $t^n := n\tau, n = 0, \dots, N$, be a uniform partition of the interval $[0, T]$. Since we consider q-step schemes, we assume that starting approximations $u^0, \dots, u^{q-1} \in V$ are given. We then recursively define a sequence of approximations $u^m \in V$ to the nodal values $u(t^m)$ of the solution u of the initial value problem (1.1) by discretizing the differential equation in (1.1) by the implicit scheme (α, β),

$$\sum_{i=0}^{q} \big(\alpha_i I + \tau \beta_i A\big) U^{n+i} = \tau \sum_{i=0}^{q} \beta_i f(t^{n+i}), \tag{1.2}$$

$n = 0, \dots, N - q$, with I the identity operator on H.

We assume that the implicit method (α, β) is A(0)-stable and denote by $\vartheta, 0 < \vartheta \leqslant 90°$, the largest angle for which the method (α, β) is A(ϑ)-stable.

The BDF methods were introduced in 1952 by two chemical engineers, Curtiss and Hirschfelder (see [5]) as *methods of forward interpolation*. The analysis of multistep methods for parabolic equations originated in [10, 11].

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1.1. **Assumptions on the linear operator A.** We denote by $(\cdot,\cdot)$ both the inner product on H and the antiduality pairing between V' and V, and by $|\cdot|$ and $\|\cdot\|$ the norms on H and V, respectively. The space V' may be considered the completion of H with respect to the dual norm $\|\cdot\|_\star$,

$$\|v\|_\star := \sup_{\substack{\tilde v\in V\\ \tilde v\neq 0}} \frac{|(v,\tilde v)|}{\|\tilde v\|} = \sup_{\substack{\tilde v\in V\\ \|\tilde v\|=1}} |(v,\tilde v)|.$$

We assume that the operator $A : V \to V'$ is *coercive* and *bounded*, i.e.,

$$\mathrm{Re}(Av,v) \geqslant \kappa\|v\|^2 \quad \forall v\in V \tag{1.3}$$

and

$$\|Av\|_\star \leqslant \nu\|v\| \quad \forall v\in V, \tag{1.4}$$

respectively, with two positive constants κ and ν. Operators satisfying (1.3) and (1.4) are sectorial in the sense that their numerical range $\{(Av,v)/(v,v), v\in V, v\neq 0\}$ is contained in a sector $S_\varphi, S_\varphi := \{z\in\mathbb{C} : z=\rho \mathrm{e}^{\mathrm{i}\psi}, \rho\geqslant 0, |\psi|\leqslant\varphi\}$, of half-angle $\varphi < 90°$.

In the analysis of non-A-stable methods, i.e., such that $\vartheta < 90°$, quantifications of the non-self-adjointness of the operator A are inevitable. There are several equivalent measures of non-self-adjointness: which measure or estimate of the non-self-adjointness of an operator is more suitable depends also on the stability technique employed; the relation between equivalent non-self-adjointness measures may be nonlinear. In the case of the energy technique, the ratio $\lambda = \nu/\kappa$ is commonly used as an estimate of the non-self-adjointness of A; notice, however, that this ratio depends on the norm $\|\cdot\|$ on V and may be a crude estimate of the non-self-adjointness of A. The ratio λ may be chosen equal to 1, if and only if the operator A is self-adjoint. A measure of the non-self-adjointness of A is, for instance, the smallest half-angle $0\leqslant\varphi<90°$ of a sector S_φ containing the numerical range of A, i.e., such that $(Av,v)\in S_\varphi$ for every $v\in V$. For alternative equivalent non-self-adjointness measures, see, for instance, [2].

1.2. **Sharp stability conditions.** A necessary stability condition for any $A(\vartheta)$-stable scheme is

$$\lambda = \frac{\nu}{\kappa} \leqslant \frac{1}{\cos\vartheta}. \tag{1.5}$$

If (1.5) holds as a strict inequality for a multistep method, then the method (1.2) is stable. The first stability proof was given by Savaré in [9]; Savaré used a Fourier stability technique, introduced by Lubich in [6].

In [2], both implicit and implicit-explicit multistep methods for *nonlinear* parabolic equations were considered. Stability was established under a sharp stability condition for implicit methods and a best possible *linear* stability condition for implicit-explicit methods by a combination of spectral and Fourier techniques. It is still not known, whether the linear stability condition for implicit-explicit methods can be relaxed if nonlinear conditions are also allowed.

1.3. **The energy technique for BDF methods.** The energy technique for high-order BDF methods is applicable via Nevanlinna–Odeh multipliers. The concept of multipliers for multistep methods was introduced by Nevanlinna and Odeh; see [8]. The energy

technique was first applied to parabolic equations by Lubich, Mansour, and Venkataraman; see [7].

In [8] multipliers of the form $(\eta_q, 0, \dots, 0)$ for the q-step BDF methods, with

$$\eta_3 = 0.0836, \quad \eta_4 = 0.2878, \quad \eta_5 = 0.8160, \tag{1.6}$$

were determined; notice that η_q cannot be replaced by a smaller number.

The smaller the sum of the absolute values of the multipliers is, the milder is the requirement on the estimate $\lambda = \nu/\kappa$ of the non-self-adjointness of A. In [4], the multipliers

$$\mu_1 = \frac{2}{169}, \quad \mu_2 = \frac{11}{169}, \quad \mu_3 = 0, \tag{1.7}$$

$$\mu_1 = \eta_4, \quad \mu_2 = \mu_3 = \mu_4 = 0, \tag{1.8}$$

and

$$\mu_1 = 0.7321818449, \quad \mu_4 = 0.07755190105, \quad \mu_2 = \mu_3 = \mu_5 = 0, \tag{1.9}$$

for the three-, four- and five-step BDF methods, respectively, were determined; it was also shown that they are optimal among the multipliers $(\mu_1, \dots, \mu_q)$, in the sense that they are the only multipliers for which the sum $\hat\eta_q := |\mu_1| + \cdots + |\mu_q|$ of the absolute values of $\mu_1, \dots, \mu_q$ attains its minimal value. While $\hat\eta_4 = \eta_4$, the new multipliers for the three- and five-step BDF methods are more favourable than the corresponding Nevanlinna–Odeh multipliers, since

$$\hat\eta_3 = \frac{1}{13} = 0.076923076 < \eta_3 = 0.0836 \quad \text{and} \quad \hat\eta_5 = 0.8097337459 < \eta_5 = 0.8160.$$

The improvement for the five-step BDF method is only minor, while for the three-step BDF method it is rather considerable.

TABLE 1.1. The sharp bounds (second column) for any stability technique, and the bounds required when Nevanlinna–Odeh (third column) or optimal (fourth column) multipliers are used in the energy technique.

q	Sharp bound: $\dfrac{1}{\cos\vartheta_q}$	NO bound: $\dfrac{1}{\eta_q}$	optimal–multipliers bound: $\dfrac{1}{\hat\eta_q}$
3	14.44374120	11.96172249	13
4	3.49010233	3.47463516	3.47463516
5	1.61849065	1.22549020	1.23497385
6	1.05051314		

For the six-step BDF method, the assumption that the operator A is selfadjoint, i.e., that $\lambda = 1$, is crucial in [3]. This could be at most relaxed to $\lambda \leqslant 1.05051314$ by any stability technique; see the last entry in the second column of Table 1.1. Since the sum of the absolute values of the multipliers exceeds 1, the assumption that the operator A is selfadjoint cannot be relaxed by the multiplier technique; it does not depend on the sum of the absolute values of the multipliers. It seems unlikely to establish stability of the six-step BDF method under a condition of the form $\lambda < \lambda^\star$ with a given, fixed $1 < \lambda^\star \leqslant 1.05051314$.

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