MODIFIED BDF METHODS FOR NONLINEAR PARABOLIC EQUATIONS

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Abstract. Implicit–explicit multistep methods for nonlinear parabolic equations are analyzed in [2] and [3]. If the implicit scheme is the $p-$step BDF, then the $p-$step implicit–explicit method of order p is stable provided the stability constant is less than $1/(2^p-1)$. Based on BDF, we construct implicit methods such that the corresponding implicit–explicit scheme of order p exhibits improved stability properties.

1. Introduction

In [2] and [3] implicit–explicit multistep schemes, and in [1] a wider class of linearly implicit methods, for nonlinear parabolic equations are analyzed. In particular, letting (α, β) be the $p-$step BDF and (α, γ) be the explicit $p-$step method of order p, it is shown in [3] that the implicit–explicit (α, β, γ) method is stable for a nonlinear parabolic equation provided the stability constant λ, see (1.4) below, is less than $1/(2^p-1)$. In this note, based on the BDF, we construct a $p-$step method $(\alpha, \tilde{\beta})$ such that the corresponding $p-$step implicit–explicit method $(\alpha, \tilde{\beta}, \gamma)$ exhibits improved stability properties for nonlinear parabolic equations. Further, we analyze general two–step second–order implicit–explicit schemes.

We consider problems of the form: Given $T > 0$ and $u^0 \in H$, find $u : [0, T] \to D(A)$ such that

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

with A a positive definite, selfadjoint, linear operator on a Hilbert space $(H, (\cdot, \cdot))$ with domain $D(A)$ dense in H, and $B(t, \cdot) : D(A) \to H$, $t \in [0, T]$, a (possibly) nonlinear operator. As a first stage in the discretization process, we consider the semidiscrete problem approximating (1.1): For a given finite dimensional subspace V_h of V, $V := D(A^{1/2})$, we seek a function u_h, $u_h(t) \in V_h$, defined by

$$\begin{cases} u_h'(t) + A_h u_h(t) = B_h(t, u_h(t)), \quad 0 < t < T, \\ u_h(0) = u_h^0; \end{cases} \tag{1.2}$$

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here $u_h^0 \in V_h$ is a given approximation to u^0, and A_h and B_h are appropriate operators on V_h with A_h a positive definite, selfadjoint, linear operator.

The time discretization of (1.2) is based on an implicit $q-$step scheme (α, β) and an explicit $q-$step scheme (α, γ), characterized by three polynomials α, β and γ,

$$\alpha(\zeta) = \sum_{i=0}^{q} \alpha_i \zeta^i , \quad \beta(\zeta) = \sum_{i=0}^{q} \beta_i \zeta^i , \quad \gamma(\zeta) = \sum_{i=0}^{q-1} \gamma_i \zeta^i .$$

For $x \in [0, \infty]$, we order the roots $\zeta_j(x)$ (resp. $\zeta_j(\infty)$), $1 \le j \le q$, of the polynomial $\varpi_x = \alpha + x\beta$ (resp. β) in such a way that the functions ζ_j are continuous in $[0, \infty]$ and that the roots $\xi_j := \zeta_j(0)$, $j = 1, \dots, s$, satisfy $|\xi_j| = 1$; these unimodular roots are called the *principal roots* of α and the complex numbers $\frac{\beta(\xi_j)}{\xi_j \alpha'(\xi_j)}$ are called the *growth factors* of ξ_j . We assume that the method (α, β) is *strongly* $A(0)-$*stable*, that means,

$$(i) \qquad \text{for all } 0 < x \le \infty \text{ and for all } j = 1, \dots, q, \text{ there holds } |\zeta_j(x)| < 1,$$

and

$$(ii) \qquad \begin{array}{c}\text{the principal roots of } \alpha \text{ are simple and their} \\ \text{growth factors have positive real parts.}\end{array}$$

Following [2], [3] and [5], and letting $N \in \mathbb{N}$, $k := \frac{T}{N}$ be the time step, and $t^n := nk, n = 0, \dots, N$, we combine the (α, β) and (α, γ) schemes to obtain an (α, β, γ) scheme for discretizing (1.2) in time, and define a sequence of fully discrete approximations U^n, $U^n \in V_h$, to $u^n := u(t^n)$, by

$$\sum_{i=0}^{q} \alpha_i U^{n+i} + k \sum_{i=0}^{q} \beta_i A_h U^{n+i} = k \sum_{i=0}^{q-1} \gamma_i B_h(t^{n+i}, U^{n+i}). \tag{1.3}$$

Given $U^0, \dots, U^{q-1}$ in $V_h, U^q, \dots, U^N$ are well defined by the (α, β, γ) scheme, see [2]. The scheme (1.3) is efficient, its implementation to advance in time requires solving a linear system with the same matrix for all time levels.

Let $|\cdot|$ denote the norm of H, and introduce in V the norm $\|\cdot\|$ by $\|v\| := |A^{1/2}v|$. We identify H with its dual, and denote by V' the dual of V, again by $(\cdot, \cdot)$ the duality pairing between V' and V, and by $\|\cdot\|_\star$ the dual norm on V', $\|v\|_\star := |A^{-1/2}v|$. Let T_u be a tube around the solution u, $T_u := \{v \in V : \min_t \|u(t) - v\| \le 1\}$, say. For stability purposes, we assume that $B(t, \cdot)$ can be extended to an operator from V into V', and an estimate of the form

$$\|B(t, v) - B(t, w)\|_\star \le \lambda \|v - w\| + \mu |v - w| \qquad \forall v, w \in T_u \tag{1.4}$$

holds, uniformly in t, with the *stability constant* λ and a constant μ. The scheme (1.3) is shown in [3] to be locally stable under the condition

$$\lambda < 1/K_{(\alpha,\beta,\gamma)} , \tag{1.5}$$

with

$$K_{(\alpha,\beta,\gamma)} := \sup_{x>0} \max_{\zeta \in S_1} \left|\frac{x\gamma(\zeta)}{(\alpha + x\beta)(\zeta)}\right| \tag{1.6}$$

and $S_1 := \{z \in \mathbb{C} : |z| = 1\}$; if the constant λ in (1.4) exceeds the right-hand side of (1.5), then the $(\alpha, \beta, \gamma)-$scheme may in general be only conditionally stable, see [3]. We refer to [3] for details for the space discretization and for error estimates.

Given an implicit $p-$step scheme (α, β) of order p, the order of the explicit $p-$step scheme (α, γ) is p, if and only if

$$\gamma(\zeta) = \beta(\zeta) - \beta_p(\zeta - 1)^p, \tag{1.7}$$

see [2].

Let now (α, β) be the $p-$step BDF,

$$\alpha(\zeta) = \sum_{j=1}^{p} \frac{1}{j}\zeta^{p-j}(\zeta - 1)^j \quad \text{and} \quad \beta(\zeta) = \zeta^p; \tag{1.8}$$

it is well known that the order of these schemes is p and that they are strongly $A(0)-$stable for $1 \le p \le 6$. Motivated by (1.7), we associate to the (α, β) BDF the explicit (α, γ) scheme with

$$\gamma(\zeta) := \zeta^p - (\zeta - 1)^p. \tag{1.9}$$

For the corresponding (α, β, γ) scheme we have

$$K_{(\alpha,\beta,\gamma)} = 2^p - 1, \tag{1.10}$$

$1 \le p \le 6$, see [3]. Our purpose in this paper is, based on the BDF, to construct $p-$step $(\alpha, \tilde{\beta}, \gamma)$ schemes of order p such that $K_{(\alpha,\tilde{\beta},\gamma)}$ be small and, in particular,

$$K_{(\alpha,\tilde{\beta},\gamma)} < K_{(\alpha,\beta,\gamma)}, \quad p = 2, \dots, 6; \tag{1.11}$$

$p = 1$ is excluded here because in this case (1.5) reads $\lambda < 1$ which, of course, cannot be relaxed. Further, for two–step second–order schemes we will also consider the general case, and will construct schemes such that $K_{(\alpha,\beta,\gamma)}$ be arbitrarily close to one.

An outline of the paper is as follows: In section 2 we present some auxiliary material. In section 3 we will modify the second–order BDF and will construct a scheme for which the stability condition will be $\lambda < 1/2$, while the corresponding condition for the BDF is $\lambda < 1/3$. In section 4 we will start from the general second–order two–step scheme and will be led to a two–parameter family of implicit–explicit schemes with very good stability properties for appropriate values of the parameters. Section 5 is devoted to modified third–order BDF. In section 6 we briefly discuss modified higher–order BDF with improved stability properties.

2. Preliminaries

In this section we present some auxiliary material that will be used in the sequel.

In the following sections, based on the $p-$step BDF (α, β) and the corresponding explicit $p-$step scheme (α, γ) of order p, described by the polynomials in (1.8) and (1.9), we shall construct implicit $p-$step schemes $(\alpha, \tilde{\beta})$ resulting to implicit–explicit $(\alpha, \tilde{\beta}, \gamma)-$schemes with improved stability properties, in particular satisfying (1.11).

For two–step second–order schemes we will both modify the second–order BDF and also consider the general case.

Our approach has been motivated by a similar construction of implicit modified BDF by Fredebeul [6]. Let us however emphasize that the two constructions lead to different schemes. Also, the goal of [6] is the construction of modified BDF per se, while we are mainly interested in the stability properties of the implicit–explicit $(\alpha, \tilde{\beta}, \gamma)$ scheme. Further, we modify the BDF by linearly combining the schemes (α, β) and (α, γ), while Fredebeul combines the scheme (α, β) with the "explicit $p-$step BDF" $(\tilde{\alpha}, \tilde{\gamma})$, $\tilde{\gamma}(\zeta) := \zeta^{p-1}$.

Let $s \in \mathbb{R}, s \neq 0, 1$. Multiplying the $p-$step BDF (α, β) by s and subtracting from the corresponding (α, γ) scheme, we are led to the implicit scheme $(\alpha, \tilde{\beta})$ with

$$\tilde{\beta} := \frac{1}{s-1}(s\beta - \gamma). \tag{2.1}$$

The order of the scheme $(\alpha, \tilde{\beta})$ is obviously at least p. Further, let the consistency constant C_{p+1} of a $p-$step scheme (α, β) of order p be defined by the relation

$$\sum_{i=0}^{p} \big[\alpha_i y(t+ik) - k\beta_i y'(t+ik)\big] = C_{p+1} k^{p+1} y^{(p+1)}(t) + O(k^{p+2})$$

for smooth functions y with bounded derivative of order $p+2$. Now, the consistency constants of the schemes (α, β) and (α, γ) are $-1/(p+1)$ and $p/(p+1)$, respectively; thus we easily conclude that the order of the scheme $(\alpha, \tilde{\beta})$ is p for $s \neq -p$, and at least $p+1$ for $s = -p$.

In the following sections our goal will be, for $p = 2, \dots, 6$, to select s in (2.1) in such a way that the scheme $(\alpha, \tilde{\beta})$ be strongly $A(0)-$stable and (1.11) be satisfied for the implicit–explicit scheme $(\alpha, \tilde{\beta}, \gamma)$.

Let us recall that a polynomial $a, a(z) = a_k z^k + \cdots + a_0$ $(a_k \neq 0)$, is called a *Schur polynomial* if all its roots lie inside the unit circle in the complex plane. Thus, condition (i) in the definition of the strong $A(0)-$stability may be rephrased as

(i) $\qquad \varpi_x$ is a Schur polynomial for all $0 < x \leq \infty$.

To check this we may use the Schur criterion or the Routh-Hurwitz criterion, which we recall here for the convenience of the reader.

Schur's criterion: Let $a, a(z) = a_k z^k + \cdots + a_0$ $(a_k \neq 0)$, be a polynomial with complex coefficients and set

$$a^\star(z) = \bar{a}_0 z^k + \cdots + \bar{a}_k,$$

and

$$\tilde{a}(z) = \frac{1}{z}[\bar{a}_k\, a(z) - a_0\, a^\star(z)].$$

Then, a is a Schur polynomial if and only if $|a_0| < |a_k|$ and $\tilde{a}$ (a polynomial of degree $k-1$) is a Schur polynomial.

Routh–Hurwitz's criterion: Let $a, a(z) = a_k z^k + \cdots + a_0$ $(a_k \neq 0)$, be a polynomial with real coefficients, set

$$A(z) := (1-z)^k\, a\Big(\frac{1+z}{1-z}\Big) = b_0 z^k + \cdots + b_k$$

and assume without loss of generality that b_0 is positive. Then, a is a Schur polynomial if and only if the roots of A have negative real parts, i.e., if and only if the Routh–Hurwitz conditions are satisfied.

For $k = 2, 3$ and 4, the Routh–Hurwitz conditions can be written in the form

$$\begin{aligned} k=2: &\quad b_i > 0,\ i = 0,1,2,\\ k=3: &\quad b_i > 0,\ i = 1,2,3, \qquad b_1b_2 - b_3b_0 > 0,\\ k=4: &\quad b_i > 0,\ i = 1,2,3,4, \quad b_1b_2b_3 - b_0b_3^2 - b_4b_1^2 > 0. \end{aligned}$$

In the following sections we will often use the $\inf_{\tau>0} |z_1 + \tau z_2|$ for given complex numbers z_1, z_2. It is easily seen that

$$\inf_{\tau>0} |z_1 + \tau z_2| = |z_1| \qquad \text{if} \quad \operatorname{Re}(z_1\bar z_2) \geq 0, \tag{2.2}$$

and

$$\inf_{\tau>0} |z_1 + \tau z_2| = |z_1 + \tau^\star z_2| = \Big(|z_1|^2 - \frac{1}{|z_2|^2}\big(\operatorname{Re}(z_1\bar z_2)\big)^2\Big)^{1/2} \quad \text{if} \quad \operatorname{Re}(z_1\bar z_2) < 0, \tag{2.3}$$

with $\tau^\star = -\frac{1}{|z_2|^2}\operatorname{Re}(z_1\bar z_2)$.

3. Modified second–order BDF

In this section our purpose is, for $p = 2$, to choose s in (2.1) in such a way that the relation $K_{(\alpha,\tilde\beta,\gamma)} < K_{(\alpha,\beta,\gamma)} = 3$ holds. Indeed, we will achieve more than this; we will see that $K_{(\alpha,\tilde\beta,\gamma)} = 2$ for $s = 3$, and $K_{(\alpha,\tilde\beta,\gamma)} > 2$ for all other values of s.

First, it is easily seen in this case that the principal root of α is 1 and its growth factor is also 1, and thus in particular positive.

Further, for a polynomial a of degree two, $a(z) = z^2 + a_1 z + a_0$, the Routh–Hurwitz conditions are

$$\begin{aligned} b_0 &= 1 - a_1 + a_0 > 0,\\ b_1 &= 2(1 - a_0) > 0,\\ b_2 &= 1 + a_1 + a_0 > 0. \end{aligned}$$

Therefore, $\varpi_{x,s}$,

$$\varpi_{x,s}(\zeta) = \Big(\frac{3}{2} + \frac{sx}{s-1}\Big)\zeta^2 - 2\Big(1 + \frac{x}{s-1}\Big)\zeta + \frac{1}{2} + \frac{x}{s-1}\,,$$

is a Schur polynomial if and only if

$$\frac{4(s-1) + (s+3)x}{3(s-1) + 2sx} > 0, \quad \frac{(s-1)(1+x)}{3(s-1) + 2sx} > 0, \quad \frac{x(s-1)}{3(s-1) + 2sx} > 0.$$

It is easily seen that these conditions are satisfied if and only if $s < -3$ or $s > 1$. Summarizing, the scheme $(\alpha, \tilde{\beta})$ is strongly $A(0)-$stable if and only if

$$s < -3 \quad \text{or} \quad s > 1.$$

Further, since $K_{(\alpha,\beta,\gamma)} = 3$, we are interested in values of the parameter s for which $K_{(\alpha,\tilde{\beta},\gamma)} < 3$. First, clearly,

$$3|1 - \frac{4}{s+3}| = \lim_{x\to\infty} |\frac{x\gamma(-1)}{(\alpha + x\tilde{\beta})(-1)}| \le K_{(\alpha,\tilde{\beta},\gamma)}. \tag{3.1}$$

Now, for $s \in (-\infty, -3)$, it is easily seen that

$$|1 - \frac{4}{s+3}| > 1,$$

and thus, in view of (3.1), $K_{(\alpha,\tilde{\beta},\gamma)} > 3$. Therefore, in the sequel we restrict our attention to the case $s \in (1, \infty)$. We will use (2.2) to show

$$\inf_{x>0} |\frac{1}{x}\alpha(\zeta) + \tilde{\beta}(\zeta)| = |\tilde{\beta}(\zeta)| \qquad \forall \zeta \in S_1. \tag{3.2}$$

For $\zeta \in S_1, \zeta = a + b\mathrm{i}$, we have

$$\overline{\alpha(\zeta)} = (3a+1)(a-1) - b(3a-2)\mathrm{i}$$

and

$$\tilde{\beta}(\zeta) = \frac{1}{s-1}\big[s(2a^2-1) + (1-2a) + 2b(sa-1)\mathrm{i}\big];$$

hence

$$\mathrm{Re}\,\big(\tilde{\beta}(\zeta)\overline{\alpha(\zeta)}\big) = \frac{s+3}{s-1}(a-1)^2 \ge 0, \tag{3.3}$$

and (3.2) follows in view of (2.2).

Now, it immediately follows from (3.2) that, for $s > 1$,

$$K_{(\alpha,\tilde{\beta},\gamma)} = \max_{\zeta\in S_1} |\frac{\gamma(\zeta)}{\tilde{\beta}(\zeta)}|. \tag{3.4}$$

Next we distinguish two cases: $1 < s \le 9$ and $s > 9$. For $1 < s \le 9$, we easily obtain from (3.4)

$$(K_{(\alpha,\tilde{\beta},\gamma)})^2 = \max_{-1\le a\le 1} f(a) \tag{3.5}$$

with

$$f(a) := \frac{5-4a}{1 + \frac{4a(a-1)}{s-1} + \frac{4(a-1)^2}{(s-1)^2}}\,.$$

Now

$$f'(a) = \frac{-4[1 + \frac{4a(a-1)}{s-1} + \frac{4(a-1)^2}{(s-1)^2}] - (5-4a)[\frac{4(2a-1)}{s-1} + \frac{8(a-1)}{(s-1)^2}]}{\big[1 + \frac{4a(a-1)}{s-1} + \frac{4(a-1)^2}{(s-1)^2}\big]^2};$$

therefore, $f'(a)$ vanishes if and only if a is such that

$$4a^2 - 10a - s + 7 = 0. \tag{3.6}$$

The discriminant of this quadratic equation, $4(4s-3)$, is positive since $s>1$. Therefore, for the solutions $a_1(s)$ and $a_2(s)$ of (3.6) we have

$$a_1(s)=\frac{10+2\sqrt{4s-3}}{8}=\frac{5+\sqrt{4s-3}}{4}>1$$

and

$$a_2(s)=\frac{5-\sqrt{4s-3}}{4}.$$

It is easily seen that

$$-1\le a_2(s)\le 1 \quad \text{for} \quad 1<s\le 9.$$

The function f is positive in $[-1,1]$, increasing in $[-1,a_2(s)]$, and decreasing in $[a_2(s),1]$. Thus

$$\max_{-1\le a\le 1} f(a)=f\left(\frac{5-\sqrt{4s-3}}{4}\right) \qquad \text{for} \quad s\in(1,9].$$

Now, let a function g be defined by

$$g(s):=f\left(\frac{5-\sqrt{4s-3}}{4}\right)=\frac{2(s-1)^2}{s\sqrt{4s-3}-3s+2}.$$

Then $g'(s)=0$ if and only if

$$(s-1)\big[(2s^2+3s-3)-(3s-1)\sqrt{4s-3}\big]=0.$$

Now

$$(2s^2+3s-3)^2=\big[(3s-1)\sqrt{4s-3}\big]^2$$

can be written in the form $4(s^4-6s^3+12s^2-10s+3)=0$, i.e., $(s-1)^3(s-3)=0$. We easily conclude that 3 is the only root of g' in $(1,9]$. Further, $g''(3)=2/9$ and thus $g(3)=4$ is the minimum value of g in $(1,9]$. Consequently, for $s\in(1,9]$,

$$K_{(\alpha,\tilde\beta,\gamma)}\ge 2$$

and equality holds only for $s=3$.

Further, it is obvious from (3.1) that $K_{(\alpha,\tilde\beta,\gamma)}>2$ for $s>9$.

Let us also note that the scheme $(\alpha,\tilde\beta)$, for $s=3$, is $A-$stable.

Summarizing, we can say that the $(\alpha,\tilde\beta,\gamma)-$scheme, for $s=3$, is described by the polynomials

$$\alpha(\zeta)=\frac{3}{2}\zeta^2-2\zeta+\frac{1}{2},\quad \tilde\beta(\zeta)=\frac{3}{2}\zeta^2-\zeta+\frac{1}{2},\quad \gamma(\zeta)=2\zeta-1;$$

for this scheme we have $K_{(\alpha,\tilde\beta,\gamma)}=2$.

The stability condition $\lambda<\frac{1}{3}$ for the $(\alpha,\beta,\gamma)-$scheme is thus relaxed by 50% to $\lambda<\frac{1}{2}$ for the $(\alpha,\tilde\beta,\gamma)-$scheme.

4. General second–order two–step schemes

In this section our purpose is to construct second–order two–step implicit–explicit schemes with better stability properties than the one of the previous section; our starting point here is the general second–order two–step scheme, i.e., we do not restrict ourselves in modifying the two–step BDF. We will be led to a two–parameter family of schemes such that $K_{(\alpha,\beta,\gamma)}$ be arbitrarily close to one for appropriate values of the parameters.

It is easily seen that the general second–order two–step scheme (α,β) is given by the polynomials

$$\begin{aligned}\alpha(\zeta) &= \zeta^2-(1+\tau)\zeta+\tau\\ \beta(\zeta) &= (\frac{1+\tau}{2}+\sigma)\zeta^2+(\frac{1-3\tau}{2}-2\sigma)\zeta+\sigma\end{aligned} \tag{4.1}$$

with arbitrary real parameters σ and τ. In particular, for $\sigma=-\frac{1+\tau}{2}$, we obtain the corresponding explicit second–order two–step scheme (α,γ) with

$$\gamma(\zeta)=\frac{3-\tau}{2}\zeta-\frac{1+\tau}{2}\,. \tag{4.2}$$

Let us also note that for $\sigma=0,\tau=\frac{1}{3}$, and for $\sigma=\tau=\frac{1}{3}$, respectively, (4.1) yields the two–step BDF and the modified two–step BDF of section 3.

First of all we will show that the $(\alpha,\beta)-$scheme given by (4.1) is strongly $A(0)-$stable if and only if

$$-1<\tau<1 \quad\text{and}\quad \sigma>-\frac{\tau}{2}\,; \tag{4.3}$$

thus, in the sequel we will restrict our attention to the case $\sigma>-1/2$. In fact, the corresponding polynomial $\varpi_x, \varpi_x=\alpha+x\beta$, for positive x, is given by

$$\varpi_x(\zeta)=\big[1+(\frac{1+\tau}{2}+\sigma)x\big]\Big[\zeta^2-\frac{(1+\tau)-(\frac{1-3\tau}{2}-2\sigma)x}{1+(\frac{1+\tau}{2}+\sigma)x}\zeta+\frac{\tau+\sigma x}{1+(\frac{1+\tau}{2}+\sigma)x}\Big]$$

and the Routh–Hurwitz conditions for ϖ_x to be a Schur polynomial can be written in the form

$$\frac{(1+\tau)+(\tau+2\sigma)x}{1+(\frac{1+\tau}{2}+\sigma)x}>0 \tag{4.4i}$$

$$\frac{(1-\tau)x}{1+(\frac{1+\tau}{2}+\sigma)x}>0 \tag{4.4ii}$$

$$\frac{(1-\tau)+\frac{1+\tau}{2}x}{1+(\frac{1+\tau}{2}+\sigma)x}>0\,. \tag{4.4iii}$$

Assuming that

$$\sigma\geq-\frac{1+\tau}{2}\,, \tag{4.5}$$

a necessary condition for (4.4ii) to hold for all positive x, we easily see that (4.4i), (4.4ii) and (4.4iii), respectively, are satisfied for all $x \in (0,\infty]$ if and only if

$$\tau \geq -1 \quad \text{and} \quad \sigma > -\frac{\tau}{2}, \tag{4.6i}$$

$$\tau < 1, \tag{4.6ii}$$

$$-1 < \tau \leq 1, \tag{4.6iii}$$

respectively. From (4.6) we are easily led to (4.3).

In the sequel we assume that σ and τ satisfy (4.3). For $\zeta \in S_1, \zeta = a + b\mathrm{i}$, it is easily seen that

$$\mathrm{Re}\,\big(\beta(\zeta)\overline{\alpha(\zeta)}\big) = (\tau+1)(\tau+2\sigma)(a-1)^2\,;$$

the right–hand side is nonnegative in view of (4.3), and using (2.2) we conclude

$$\inf_{x>0} |\frac{1}{x}\alpha(\zeta) + \beta(\zeta)| = |\beta(\zeta)| \qquad \forall \zeta \in S_1,$$

and thus

$$K_{(\alpha,\beta,\gamma)} = \max_{\zeta\in S_1} |\frac{\gamma(\zeta)}{\beta(\zeta)}|\,. \tag{4.7}$$

From (4.7) we easily obtain

$$(K_{(\alpha,\beta,\gamma)})^2 = 2 \max_{-1\leq a\leq 1} f(a) \tag{4.8}$$

with

$$f(a) := \frac{(\tau-3)(\tau+1)a + (\tau^2-2\tau+5)}{(\tau+1)^2(1-a^2) + [(1+\tau+4\sigma)a + 1 - 3\tau - 4\sigma]^2}\,.$$

First of all we have

$$f(1) = \frac{1}{2} \quad \text{and} \quad f(-1) = \frac{1}{2(\tau+2\sigma)^2}. \tag{4.9}$$

Let us now consider the case $\sigma = 0$; then, according to (4.3), $0 < \tau < 1$. It is easily seen that f is decreasing in $(-1,1)$ in this case. Therefore, from (4.8) and (4.9) we obtain

$$K_{(\alpha,\beta,\gamma)} = \frac{1}{\tau} \quad \text{for} \quad \sigma = 0,\ 0 < \tau < 1. \tag{4.10}$$

Consequently, for $\sigma = 0$ and τ less but close to one, the $(\alpha,\beta,\gamma)-$scheme described by (4.1) and (4.2) has excellent stability properties. Let us also note that, for $\tau = \frac{1}{3}$, relation (4.10) yields the result (1.10) for the second–order implicit–explicit BDF scheme.

Remark 4.1. A disadvantage of the $(\alpha,\beta)-$scheme described by (4.1) for $\sigma = 0$ and $0 < \tau < 1$ is that its *error constant* deteriorates as τ approaches one. Indeed the error constant of the scheme is given by

$$C = -\frac{1}{12}\frac{1+5\tau}{1-\tau}, \tag{4.11}$$

see (2.13) on page 320 of [7] for the definition. Notice, however, that for $\tau = 0.9$, say, the $(\alpha,\beta,\gamma)-$scheme has very good stability properties, the stability condition being

$\lambda < 0.9$ in this case, and the error constant of the $(\alpha,\beta)-$scheme is of moderate size, namely $C = -29/24$. Similar comments can be made for nonvanishing σ. □

Next we focus on the case $\sigma \neq 0$. In this case $f'(a) = 0$ can be written in the form

$$\sigma(3-\tau)(\tau+1)(1+\tau+2\sigma)a^2 - 2\sigma(\tau^2-2\tau+5)(1+\tau+2\sigma)a + 2t^4$$
$$+ 6\tau^2\sigma^2 - 15\sigma\tau^2 + 7\sigma\tau^3 - 4\tau^3 - 12\tau\sigma^2 + 13\sigma\tau - 2 + 4\tau + 3\sigma + 14\sigma^2 = 0$$

or equivalently

$$\begin{aligned} &\sigma(3-\tau)(\tau+1)a^2 - 2\sigma(\tau^2-2\tau+5)a \\ &\quad + 2\tau^3 - 6\tau^2 + 6\tau - 2 + 7\sigma - 6\sigma\tau + 3\sigma\tau^2 = 0. \end{aligned} \tag{4.12}$$

The discriminant $D(\sigma,\tau)$ of the quadratic equation (4.12) is given by

$$D(\sigma,\tau) = 2\sigma(\tau-1)^3[(\tau+1)(\tau-3) + 2\sigma(\tau-1)].$$

Let

$$\varphi(\tau) := (\tau+1)(\tau-3) + 2\sigma(\tau-1).$$

The roots τ_1, τ_2 of φ are

$$\tau_{1,2} = 1 - \sigma \pm \sqrt{\sigma^2+4}.$$

It is easily seen that $\tau_1 > 1$; further, $\tau_2 < -1$ for $\sigma > 0$, and $\tau_2 < -2\sigma$ for $-\frac{1}{2} < \sigma < 0$. Therefore we distinguish two cases:

First case: $-\frac{1}{2} < \sigma < 0$. In this case φ, and consequently also $D(\cdot,\sigma)$, is negative in $(-2\sigma, 1)$. It is then easily seen that f is decreasing in $(-1,1)$, and from (4.8) and (4.9) we conclude

$$K_{(\alpha,\beta,\gamma)} = \frac{1}{\tau+2\sigma} \quad \text{for} \quad -\frac{1}{2} < \sigma < 0 \quad \text{and} \quad -2\sigma < \tau < 1. \tag{4.13}$$

Obviously, for σ close to 0 and τ close to 1, the value of $K_{(\alpha,\beta,\gamma)}$ is close to one, but of course larger than one. Also, as σ tends to $-1/2$, and consequently τ tends to one, $K_{(\alpha,\beta,\gamma)}$ tends to ∞.

Second case: $\sigma > 0$. In this case $D(\cdot,\sigma)$ is positive in $(-1,1)$, and f' has two real roots a_1 and a_2,

$$a_{1,2} = \frac{\sigma(\tau^2-2\tau+5) \pm (1-\tau)\sqrt{2\sigma(\tau-1)[(\tau+1)(\tau-3)+2\sigma(\tau-1)]}}{\sigma(3-\tau)(\tau+1)}. \tag{4.14}$$

Now, $\tau^2 - 2\tau + 5 > (3-\tau)(\tau+1)$ can be written in the form $(\tau-1)^2 > 0$, which is satisfied, and we easily see that $a_1 > 1$. Further, $a_2 < 1$ can be equivalently written in the form $(\tau+1)(3-\tau) > 0$, which is, of course, valid. Further, $a_2 > -1$ can be written as

$$2\sigma(\tau^2-2\tau+5) > (1-\tau)^3. \tag{4.15}$$

Now, for $\sigma \le \psi(\tau) := (1-\tau)^3/[2(\tau^2-2\tau+5)]$, (4.15) is not satisfied, and we easily conclude

$$K_{(\alpha,\beta,\gamma)} = \max(1, \frac{1}{\tau+2\sigma}). \tag{4.16}$$

In view of (4.3) in this case we have

$$\begin{aligned} &-1<\tau<0, \quad -\frac{\tau}{2}<\sigma\le\psi(\tau)\\ \text{or}\quad &0<\tau<1, \quad 0<\sigma\le\psi(\tau)\,. \end{aligned} \tag{4.17}$$

Now, for τ and σ satisfying (4.17), it is easily seen that

$$\tau+2\sigma<\frac{\tau^2+2\tau+1}{\tau^2-2\tau+5}<1,$$

and thus (4.16) reads

$$K_{(\alpha,\beta,\gamma)}=\frac{1}{\tau+2\sigma}. \tag{4.16$'$}$$

Let us also note that when τ tends to one, $\tau+2\sigma$, and consequently also $K_{(\alpha,\beta,\gamma)}$, tends to one.

Further, obviously,

$$K_{(\alpha,\beta,\gamma)}=\max\Big(1,\frac{1}{\tau+2\sigma},\sqrt{2f(a_2)}\Big), \quad -1<\tau<1, \quad \sigma>\psi(\tau)\,, \tag{4.18}$$

with a_2 given by (4.14) (with the minus sign).

5. Modified third–order BDF

In this section our purpose is, for $p=3$, to select s in (2.1) in such a way that the relation

$$K_{(\alpha,\tilde\beta,\gamma)}<K_{(\alpha,\beta,\gamma)} \tag{5.1}$$

holds. Indeed, we will see that, for $s=9$, $K_{(\alpha,\tilde\beta,\gamma)}<5$, while $K_{(\alpha,\beta,\gamma)}=7$.

First, it is easily seen that a necessary condition for (5.1) to hold is $s>-3$. Indeed, setting

$$\tilde K_{(\alpha,\tilde\beta,\gamma)}:=\lim_{x\to\infty}\Big|\frac{x\gamma(-1)}{(\alpha+x\tilde\beta)(-1)}\Big|$$

we obviously have $\tilde K_{(\alpha,\tilde\beta,\gamma)}\le K_{(\alpha,\tilde\beta,\gamma)}$. Now

$$\tilde K_{(\alpha,\tilde\beta,\gamma)}=7\Big|\frac{s-1}{s+7}\Big|. \tag{5.2}$$

In view of (1.10) and (5.2), the relation (5.1) can only hold if $|\frac{s-1}{s+7}|<1$, i.e., $0<\frac{8}{s+7}<2$, i.e., $s>-3$.

Therefore, throughout this section we will assume that $s>-3$. Next, we will show that the scheme $(\alpha,\tilde\beta)$ is strongly $A(0)-$stable if and only if $s>2$.

In this case we have $\alpha(\zeta)=\frac{1}{6}(\zeta-1)(11\zeta^2-7\zeta+2)$, the only principal root of α is 1 and its growth factor is also equal to 1, and thus in particular positive. Therefore, it remains to show that all roots of the polynomial $\varpi_{x,s}$, $\varpi_{x,s}=\alpha+x\tilde\beta$, lie in the interior of the unit disc in the complex plane, for all positive x, if and only if $s>2$.

Let us first consider the case $x = \infty$. We claim that $\pi, \pi := s\beta - \gamma$, is a Schur polynomial (for $s > -3$) if and only if $s > 2$. We have

$$\pi(\zeta) = s\zeta^3 - 3\zeta^2 + 3\zeta - 1,$$

and, according to Schur's criterion, a necessary condition for π to be a Schur polynomial is $|s| > 1$, i.e.,

$$s < -1 \quad \text{or} \quad s > 1. \tag{5.3}$$

Further, to apply Schur's criterion, let $\pi^\star$ be given by $\pi^\star(\zeta) := -\zeta^3 + 3\zeta^2 - 3\zeta + s$. Then,

$$\pi^\star(0)\pi(\zeta) - \pi(0)\pi^\star(\zeta) = (s-1)[(s+1)\zeta^3 - 3\zeta^2 + 3\zeta].$$

Consider now the polynomial π_1, $\pi_1(\zeta) = (s+1)\zeta^2 - 3\zeta + 3$. For π_1 to be a Schur polynomial we must have $|s+1| > 3$, i.e., $s < -4$ or $s > 2$, and therefore, since we have assumed that $s > -3$, we must have $s > 2$. Moreover, with $\pi_1^\star$, $\pi_1^\star(\zeta) := 3\zeta^2 - 3\zeta + (s+1)$, we have

$$\pi_1^\star(0)\pi_1(\zeta) - \pi_1(0)\pi_1^\star(\zeta) = (s-2)[(s+4)\zeta^2 - 3\zeta].$$

Consider then π_2, $\pi_2(\zeta) := (s+4)\zeta - 3$. This is a Schur polynomial for $s > -1$ or $s < -7$. Summarizing, $s\beta - \gamma$ is a Schur polynomial for $s > 2$; (actually this is also the case for $s < -7$, but as already emphasized we are here only interested in values of s larger than -3).

Next, we want to show that, for $x > 0$, $\varpi_{x,s}$, $\varpi_{x,s} := \alpha + x\tilde{\beta}$, is a Schur polynomial for $s > 2$. We have

$$\varpi_{x,s}(\zeta) = (\frac{11}{6} + \frac{sx}{s-1})\zeta^3 - 3(1 + \frac{x}{s-1})\zeta^2 + 3(\frac{1}{2} + \frac{x}{s-1})\zeta - (\frac{1}{3} + \frac{x}{s-1})\,.$$

First, obviously, for the values of s and x under consideration,

$$\frac{1}{3} + \frac{x}{s-1} < \frac{11}{6} + \frac{sx}{s-1}\,.$$

Further, to apply Schur's criterion, let $\varpi_{x,s}^\star$, be given by

$$\varpi_{x,s}^\star(\zeta) := -(\frac{1}{3} + \frac{x}{s-1})\zeta^3 + 3(\frac{1}{2} + \frac{x}{s-1})\zeta^2 - 3(1 + \frac{x}{s-1})\zeta + (\frac{11}{6} + \frac{sx}{s-1})\,.$$

Then,

$$\begin{aligned}
&\varpi_{x,s}^\star(0)\varpi_{x,s}(\zeta) - \varpi_{x,s}(0)\varpi_{x,s}^\star(\zeta) = \\
&\quad = \frac{1}{s-1}\Big[\Big(\frac{13(s-1)}{4} + \frac{11s-2}{3}x + (s+1)x^2\Big)\zeta^3 \\
&\qquad - 3\Big(\frac{5(s-1)}{3} + (s+1)x + x^2\Big)\zeta^2 + 3\Big(\frac{7(s-1)}{12} + \frac{s+1}{2}x + x^2\Big)\zeta\,.
\end{aligned}$$

Consider then the polynomial π,

$$\begin{aligned}
\pi(\zeta) := &\Big(\frac{13(s-1)}{4} + \frac{11s-2}{3}x + (s+1)x^2\Big)\zeta^2 \\
&- 3\Big(\frac{5(s-1)}{3} + (s+1)x + x^2\Big)\zeta + 3\Big(\frac{7(s-1)}{12} + \frac{s+1}{2}x + x^2\Big)\,.
\end{aligned}$$

First, obviously, for the values of s and x under consideration,

$$3\big(\frac{7(s-1)}{12}+\frac{s+1}{2}x+x^2\big)<\frac{13(s-1)}{4}+\frac{11s-2}{3}x+(s+1)x^2\,.$$

Further, to apply Schur's criterion, let $\pi^\star$ be given by

$$\begin{aligned}\pi^\star(\zeta)&:=3\big(\frac{7(s-1)}{12}+\frac{s+1}{2}x+x^2\big)\zeta^2\\&\quad-3\big(\frac{5(s-1)}{3}+(s+1)x+x^2\big)\zeta+\big(\frac{13(s-1)}{4}+\frac{11s-2}{3}x+(s+1)x^2\big)\,.\end{aligned}$$

Then,

$$\begin{aligned}\pi^\star(0)\pi(\zeta)-\pi(0)\pi^\star(\zeta)&=[\frac{3}{2}(s-1)+\frac{13}{6}(s-1)x+(s-2)x^2]\times\\&\Big[[5(s-1)+\frac{31s+5}{6}x+(s+4)x^2]\zeta^2-[5(s-1)+3(s+1)x+3x^2]\zeta\Big]\,.\end{aligned}$$

It is easily seen that this is a Schur polynomial for the values of s and x under consideration.

Now, let

$$\begin{aligned}S_1^+&:=\{z\in S_1:\mathrm{Re}\,\big(\tilde\beta(\zeta)\overline{\alpha(\zeta)}\big)\geq 0\},\\S_1^-&:=\{z\in S_1:\mathrm{Re}\,\big(\tilde\beta(\zeta)\overline{\alpha(\zeta)}\big)<0\}.\end{aligned}$$

Then, in view of (2.2) and (2.3),

$$\forall\zeta\in S_1^+\qquad\sup_{x>0}\,|\frac{x\gamma(\zeta)}{(\alpha+x\tilde\beta)(\zeta)}|=|\frac{\gamma(\zeta)}{\tilde\beta(\zeta)}|,\tag{5.4}$$

$$\forall\zeta\in S_1^-\quad\sup_{x>0}\,|\frac{x\gamma(\zeta)}{(\alpha+x\tilde\beta)(\zeta)}|=\frac{|\gamma(\zeta)|}{\Big(|\tilde\beta(\zeta)|^2-\frac{1}{|\alpha(\zeta)|^2}\big(\mathrm{Re}(\tilde\beta(\zeta)\overline{\alpha(\zeta)})\big)^2\Big)^{1/2}}.\tag{5.5}$$

Hence, letting

$$K_3^+:=\max_{\zeta\in S_1^+}|\frac{\gamma(\zeta)}{\tilde\beta(\zeta)}|,$$

and

$$K_3^-:=\max_{\zeta\in S_1^-}\frac{|\gamma(\zeta)|}{\Big(|\tilde\beta(\zeta)|^2-\frac{1}{|\alpha(\zeta)|^2}\big(\mathrm{Re}(\tilde\beta(\zeta)\overline{\alpha(\zeta)})\big)^2\Big)^{1/2}},$$

we easily conclude

$$K_{(\alpha,\tilde\beta,\gamma)}=\max(K_3^+,K_3^-).\tag{5.6}$$

We have computed K_3^+ and K_3^- for various values of s; according to our computations one reasonable choice for s seems to be $s=9$. For this s we have $K_3^+\approx 4.82893515$ and $K_3^-\approx 2.85220717$; therefore, it is safe to say that

$$K_{(\alpha,\tilde\beta,\gamma)}<5\quad\text{for}\quad s=9.\tag{5.7}$$

6. Modified higher–order BDF

In this section we will construct modified fourth–, fifth– and sixth–order BDF such that the corresponding implicit–explicit schemes exhibit improved stability properties.

We will use notation analogous to the one of the previous Section.

First, for $p = 4$, we have $K_{(\alpha,\beta,\gamma)} = 15$, while for $s = 26$, which is a reasonable choice according to our computations, we have $K_4^+ \approx 10.9366302$ and $K_4^- \approx 8.48358536$, and it is thus safe to say that

$$K_{(\alpha,\tilde{\beta},\gamma)} < 11 \quad \text{for} \quad s = 26. \tag{6.1}$$

Similarly, for $p = 5$ and $p = 6$ we have computed

$$K_5^+ \approx 23.7191849, \quad K_5^- \approx 21.0605831 \quad \text{for} \quad s = 68$$

and

$$K_6^+ \approx 50.1196861, \quad K_6^- \approx 48.4871178 \quad \text{for} \quad s = 168,$$

respectively, and thus we can say that, for $p = 5$,

$$K_{(\alpha,\tilde{\beta},\gamma)} < 24 \quad \text{for} \quad s = 68, \tag{6.2}$$

while $K_{(\alpha,\beta,\gamma)} = 31$, and, for $p = 6$,

$$K_{(\alpha,\tilde{\beta},\gamma)} < 51 \quad \text{for} \quad s = 168, \tag{6.3}$$

while $K_{(\alpha,\beta,\gamma)} = 61$.

Let us mention that we have checked the schemes $(\alpha, \tilde{\beta})$ mentioned in (6.1), (6.2) and (6.3) and found them to be strongly $A(0)-$stable.

References

[1] G. Akrivis and M. Crouzeix *Linearly implicit methods for nonlinear parabolic equations*, Math. Comp. (to appear).

[2] G. Akrivis, M. Crouzeix and Ch. Makridakis, *Implicit-explicit multistep finite element methods for nonlinear parabolic problems*, Math. Comp. **67** (1998) 457–477.

[3] G. Akrivis, M. Crouzeix and Ch. Makridakis, *Implicit-explicit multistep methods for quasilinear parabolic equations*, Numer. Math. **82** (1999) 521–541.

[4] G. Akrivis, O. Karakashian and F. Karakatsani, *Linearly implicit methods for nonlinear evolution equations*, Numer. Math. **94** (2003) 403–418.

[5] M. Crouzeix, *Une méthode multipas implicite-explicite pour l'approximation des équations d'évolution paraboliques*, Numer. Math. **35** (1980) 257–276.

[6] Ch. Fredebeul, *A-BDF: A generalization of the backward differentiation formulae*, SIAM J. Numer. Anal. **35** (1998) 1917–1938.

[7] E. Hairer, S. P. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I: Nonstiff Problems.* Springer–Verlag, Berlin Heidelberg, Springer Series in Computational Mathematics v. 8, 1987.

[8] E. Hairer, G. Wanner, *Solving Ordinary Differential Equations II: Stiff and Differential–Algebraic Problems.* Springer–Verlag, Berlin Heidelberg, Springer Series in Computational Mathematics v. 14, 1991.

[9] J. D. Lambert, *Numerical Methods for Ordinary Differential Systems.* John Wiley & Sons, Baffins Lane, Chichester, West Sussex, 1991.

[10] V. Thomée, *Galerkin Finite Element Methods for Parabolic Problems.* Springer–Verlag, Berlin, Springer Series in Computational Mathematics v. 25, 1997.

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