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Second order Chebyshev methods based on orthogonal polynomials

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Summary. Stabilized methods (also called Chebyshev methods) are explicit Runge-Kutta methods with extended stability domains along the negative real axis. These methods are intended for large mildly stiff problems, originating mainly from parabolic PDEs. The aim of this paper is to show that with the use of orthogonal polynomials, we can construct nearly optimal stability polynomials of second order with a three-term recurrence relation. These polynomials can be used to construct a new numerical method, which is implemented in a code called ROCK2. This new numerical method can be seen as a combination of van der Houwen-Sommeijer-type methods and Lebedev-type methods.

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1 Introduction

The integration of initial value problems of differential equations is usually done by *explicit* methods (in the non-stiff case) or by *implicit* methods in the stiff case. The latter have the advantage of being unconditionally stable, but the disadvantage that they need the solution of implicit equations, which can cost a considerable amount of computations, especially for high dimensional problems.

In many situations, namely when the stiffness is “mild”, the dimension is high and the eigenvalues of the Jacobian matrix are known to be in a long

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narrow strip along the negative real axis, *stabilized explicit Runge-Kutta methods* (which are a compromise between the two precedent methods), are very efficient. These methods possess large stability domains along the negative real axis. The good performance of such explicit methods for stiff problems is mainly due to the property that the size of the stability domain, along the negative real axis, increases *quadratically* with the stage number. A typical application of such methods is the time integration of parabolic PDEs converted by the method of lines into a system of ODEs.

Up to now, there exist two types of second order stabilized explicit methods:

a) *Lebedev-type methods*, which have the advantage that the stability polynomials are optimal. But there is no recurrence relation, and an appropriate ordering of the zeros is needed for ensuring stability properties of the numerical method (see [9,10,13]).

b) *Van der Houwen-Sommeijer methods*, based on a linear combination of shifted Chebyshev polynomials. Here the advantage is the three-term recurrence relation of Chebyshev polynomials, which can be used to construct the numerical method. But the stability region on the negative real axis is only about 80% of the optimal interval (see [8]).

For more details concerning these two approaches we refer to [6, pp. 31–36] and [17].

In this paper we discuss a method which combines the advantages of the two precedent methods in the following way. We search for polynomials which possess:

1. Second order accuracy;
2. A three-term recurrence relation;
3. A nearly optimal stability interval.

This will allow us to derive new stabilized Runge-Kutta methods.

The paper is organized as follows: In Sect. 2, we motivate our strategy with the help of a theorem of Bernstein. In Sect. 3, we explain how to construct the stability functions based on orthogonal polynomials, and give in Sect. 4 results on existence and on the error constants of the constructed stability polynomials. In Sect. 5, we show how to compute numerically the recurrence coefficients of the polynomials. We describe in Sect. 6 the construction of the numerical method based on a three-term recurrence relation, implemented in a code called ROCK2 (for second order Orthogonal-Runge-Kutta-Chebyshev, appropriately permuted to make it sound more solid). Finally, Sect. 7 contains numerical experiments with ROCK2 and comparisons with the code RKC of Sommeijer, Shampine and Verwer [15], based on van der Houwen-Sommeijer methods.

2 From optimal stability polynomials to orthogonal polynomials

We start from the optimal stability polynomials of second order (i.e. $\mathrm{e}^z - R_s(z) = \mathcal{O}(z^3)$), upon which the Lebedev-type algorithm is based[1]:

$$
(1) \qquad \begin{aligned} &\bar{R}_s(z) = 1 + z + \tfrac{z^2}{2!} + \textstyle\sum_{i=3}^{s} \alpha_{i,s} z^i, \text{with } \alpha_{i,s} \in \mathbb{R}, \\ &|\bar{R}_s(z)| \leq 1 \quad \text{for} \quad z \in [-\bar{l}_s, 0] \quad \text{with } \bar{l}_s \text{ as large as possible.} \end{aligned}
$$

We know (see [14]) that such polynomials exist and are unique (for all orders and degrees). These polynomials satisfy an equal ripple property on $s-1$ points, i.e. there exist $-\bar{l}_s = z_0 < z_1 < z_2 < \ldots < z_{s-2} < 0$ such that

$$
(2) \qquad \begin{aligned} &\bar{R}_s(z_i) = -\bar{R}_s(z_{i+1}) \qquad \forall i = 0, \ldots, s-3 \\ &|\bar{R}_s(z_i)| = 1 \qquad\qquad\quad\;\; \forall i = 0, \ldots, s-2. \end{aligned}
$$

These polynomials possess exactly 2 complex zeros. A description of the zeros and the error constant of these polynomials (for all orders and degrees) is given in [1]. It is desirable in practice to replace (1) by $|\bar{R}_s(z)| \leq \eta < 1$ (damping), where ϵ is a small positive parameter. The stability domains become a bit shorter, but a small strip around the negative real axis is included in the stability region. Throughout this paper we will choose $\eta = 0.95$.

Remark 1. No *explicit* analytical solutions are known for second order optimal stability polynomials. Analytic expressions in terms of an elliptic integral have been obtained by Lebedev [11]. In practice their computation is done numerically [10, 13].

Example 1. For order 1, the optimal polynomials are $T_s(1 + \frac{z}{s^2})$, the shifted Chebyshev polynomials. They satisfy an equal ripple property and a condition similar to (1) (for order 1) with $\bar{l}_s = 2s^2$ (see Fig. 1). The Chebyshev polynomials (shifted in $[-1, 1]$) are at the same time orthogonal polynomials associated with the weight function $1/\sqrt{(1-x^2)}$. Thus, for order 1, optimal stability polynomials are orthogonal polynomials.

Inspired by Example 1 we try, for order 2, to find an approximation of optimal stability polynomials involving orthogonal polynomials. As we will use orthogonal polynomials on $[-1, 1]$, we shift $\bar{R}_s(z)$ in this interval (by setting $x = 1 + \frac{2z}{\bar{l}_s}$) and write it as (using the same notation for the shifted polynomial)

$$
(3) \qquad \bar{R}_s(x) = \bar{w}(x)\bar{P}_{s-2}(x),
$$

[1] We use the notation $\bar{R}_s$ because we reserve R_s for the stability polynomials we will construct in Sect. 3

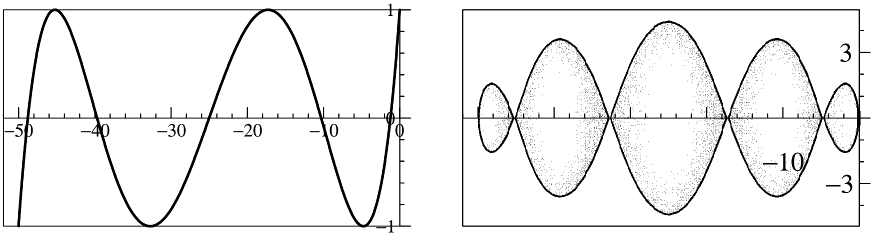

Fig. 1. A shifted Chebyshev polynomial and its stability domain (s=5)

where $\bar{w}(x)$ is a polynomial of degree 2 (depending on s) which possesses the 2 complex zeros of $\bar{R}_s(x)$. As $\bar{R}_s(1) = 1$, we will suppose that $\bar{w}(1) = \bar{P}_{s-2}(1) = 1$. The order and the stability conditions (1) can be written in the interval $[-1, 1]$ as

$$\bar{R}_s(1) = 1, \quad \bar{R}_s'(1) = \bar{d}_s, \quad \bar{R}_s''(1) = \bar{d}_s^{\,2}. \tag{4}$$

where $\bar{d}_s = \bar{l}_s/2$, and

$$\max_{x\in[-1,1]} |\bar{R}_s(x)| = 1. \tag{5}$$

In order to introduce orthogonal polynomials we consider a minimization problem. Among all polynomials of degree $s-2$ equal to 1 at $x = 1$ (normalization), the polynomial $\bar{P}_{s-2}(x)$ of (3) satisfies

$$\max_{x\in[-1,1]} |\bar{w}(x)\bar{P}_{s-2}(x)| \longrightarrow \min, \tag{6}$$

where $\bar{w}(x)$ is the polynomial defined above. Indeed, suppose that a polynomial $Q(x)$ of degree $s-2$ equal to 1 at $x = 1$ is a solution of equation (6). Then, due to the equal ripple property (2) of $\bar{w}(x)\bar{P}_{s-2}(x)$ and the normalization, the difference

$$\bar{w}(x)(\bar{P}_{s-2}(x) - Q(x))$$

has $s-1$ zeros not at the origin. Thus $Q(x) \equiv \bar{P}_{s-2}(x)$ since $\bar{w}(x)$ has only complex zeros.

After having formulated this minimization problem, the motivation for constructing a stability function involving orthogonal polynomials comes from a theorem of Bernstein. Let us state this theorem (see [2] or [16, p. 290] for a proof):

Theorem 1. *[2] Let $q(x)$ be a positive weight function on the interval $[-1, 1]$ which satisfies $0 < \lambda < q(x) < \Lambda$ and $|q(x+\delta) - q(x)||\ln\delta|^{1+\epsilon} < L$ (where $\lambda, \Lambda, \epsilon, L$ are fixed positive numbers).*

Then the orthogonal polynomials $P_n(x)$ associated with the weight function $q(x)/(\sqrt{1-x^2})$, satisfy uniformly on $[-1, 1]$:

$$q(x)^{1/2}P_n(x) = \cos(n\theta + \psi(\theta)) + \mathcal{O}(\ln(n)^{-\epsilon}), \quad \theta = \arccos(x). \tag{7}$$

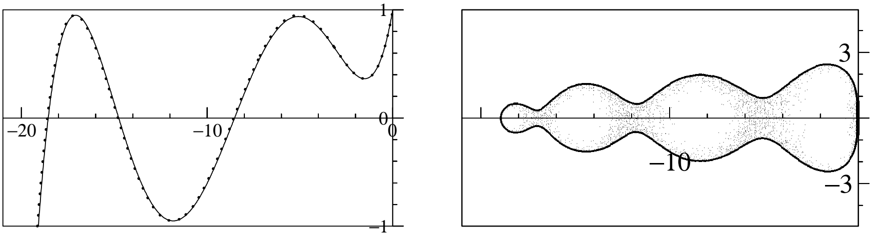

Fig. 2. $R_5(x)$ (shifted) and its stability domain, with $\bar{R}_5(x)$ in dotted line, $\eta = 0.95$ (damping)

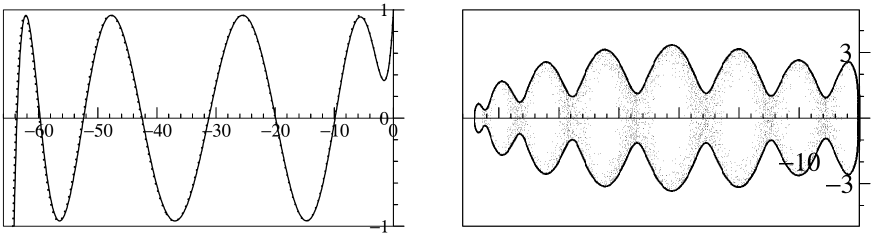

Fig. 3. $R_9(x)$ (shifted) and its stability domain, with $\bar{R}_9(x)$ in dotted line, $\eta = 0.95$ (damping)

where $\psi(\theta) = \frac{1}{2\pi} \int_{-1}^{1} \frac{\ln q(z) - \ln q(x)}{z - x} \sqrt{\frac{1-x^2}{1-z^2}} dz.$

The function $\psi(\theta)$ is called the Szegö-Bernstein phase function. Under the preceding assumptions it is continuous and satisfies $\psi(0) = \psi(\pi) = 0$ (again see [2]).

If we set $q(x) = \bar{w}(x)^2$ and $n = s - 2$, then formula (7) shows that with an accuracy of $\mathcal{O}(\ln(n)^{-\epsilon})$, $\bar{w}(x)P_{s-2}(x)$ alternates (with absolute value 1) on $s - 1$ points of $[-1, 1]$. Thus, it is asymptotically a solution of (6).

Our idea is to use the orthogonal polynomial $P_{s-2}(x)$ instead of $\bar{P}_{s-2}(x)$. More precisely, we want to find:

- $w(x)$ a positive polynomial of degree 2 (depending on s);
- $P_{s-2}(x)$, an orthogonal polynomial associated with the weight function $w(x)^2/(\sqrt{1-x^2})$ such that

$$R_s(x) = w(x)P_{s-2}(x)$$

  results in a second order stability polynomial, which remains bounded as long as possible on the negative real axis (see Figs. 2 and 3, the optimal polynomial and its approximation are very close).

For a given s, we will then construct a family of orthogonal polynomials associated with the computed weight function $w(x)^2/(\sqrt{1-x^2})$. These polynomials denoted by $P_j(x)$ $(j = 0, \ldots, s-2)$ possess a three-term recurrence relation which will be used to define the numerical method.

3 The stability polynomials

In this section we will explain how to construct our stability polynomials. Given a degree $s \geq 3$, let $w(x) = (x - (\alpha + i\beta))(x - (\alpha - i\beta))$ and let $P_{s-2}(x)$ be the orthogonal polynomial on $[-1, 1]$ of degree $s - 2$, associated with the weight function $w(x)^2/\sqrt{1 - x^2}$. If we normalize the polynomial $w(x)P_{s-2}(x)$ such that $|w(x)P_{s-2}(x)| \leq 1$ for $x \in [-1, 1]$, then $w(1)P_{s-2}(1)$ is usually different from 1. Therefore, we introduce a parameter a close to 1, set

$$R_s(x) = \frac{w(x)P_{s-2}(x)}{w(a)P_{s-2}(a)}, \tag{8}$$

and we search second order conditions at the point a.

We will use sometimes the notation $R_s(x, \alpha, \beta)$ which emphasizes the dependence of $R_s(x)$ on α and β. Since $w(x)$ depends quadratically on β, we will restrict ourselves to parameters $\beta \geq 0$. We emphasize that not only $w(x)$ but also $P_{s-2}(x)$ depends on α and β in a non-linear way via the orthogonality condition. In Sect. 4 we will show that for α and β in a certain region the non-linear equations (9) below have a solution.

Problem: find a, d, α, β such that

$$R_s'(a, \alpha, \beta) = d, \quad R_s''(a, \alpha, \beta) = d^2 \tag{9}$$

$$|R_s(x)| \leq 1 \quad x \in [-1, a] \tag{10}$$

$$l = (1 + a)d \quad \text{as large as possible.} \tag{11}$$

Then, if we set $z = (x - a)d$ and denote by $\hat{R}_s(z) = R_s(a + z/d)$ the shifted polynomial, we have

$$\hat{R}_s(0) = 1 \quad \hat{R}_s'(0) = 1, \quad \hat{R}_s''(0) = 1 \tag{12}$$

$$|\hat{R}_s(z)| \leq 1 \quad z \in [-l, 0]. \tag{13}$$

To compute the parameters a, d, α, β, we will proceed in two steps:

1) Given a and d we have to determine $\alpha_{new}, \beta_{new}$ such that (9) is satisfied. This is a system of non-linear equations

$$\begin{aligned} R_s'(a, \alpha_{new}, \beta_{new}) &= d \\ R_s''(a, \alpha_{new}, \beta_{new}) &= d^2. \end{aligned} \tag{14}$$

Numerical computations show that for a and $d \neq 0$ given, the solutions of (14) are locally unique, thus we can solve the two non-linear equations by an iterative method. We will show in Sect. 5 that there exist explicit formulas for

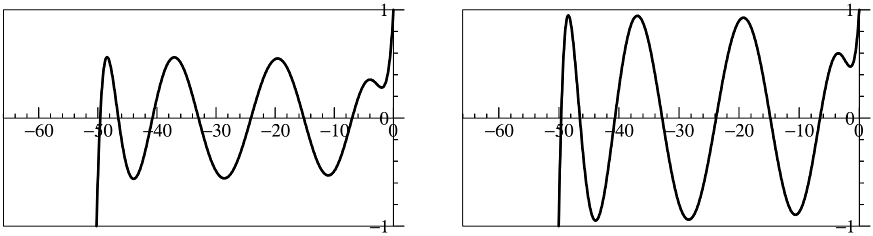

Fig. 4. Approximation polynomials (shifted) of degree 9 with $a_{old} = 1.01$ (left), $a_{new} = 0.99$ (right), $\eta = 0.95$ (damping)

the polynomial $R_s(x)$ and its derivatives which can be used for the iterative method.

2) Given a second order polynomial $R_s(x)$ we will compute a_{new} such that (10) is satisfied and optimize the parameter l of (11).

i) Computation of a_{new}.

The second order polynomial $R_s(x)$ given by equations (14) does not necessarily satisfy

$$\max_{x \in [-1, a-\epsilon]} |R_s(x)| = 1, \tag{15}$$

where $\epsilon > 0$ is the smallest number such that $R_s(x)$ has a local extremum at $a - \epsilon$. We set $a = a_{old}$ and we search a_{new} such that (15) is satisfied (see Fig. 4).

This can be done in the following way:

let $m = \max_{x \in [-1, a_{old}-\epsilon]} |R_s(x)|$;
• if $m > 1$ we search $a_{new} > a_{old}$ such that $R_s(a_{new}) = m$;
• if $m < 1$ we search $a_{new} < a_{old}$ such that $R_s(a_{new}) = m$.

Since $R_s(x)$ is increasing for $a > \max(\alpha, \gamma_{s-2})$, where γ_{s-2} is the largest zero of $R_s(x)$, and since $R_s(x)$ is decreasing if a tends to γ_{s-2}, it is always possible to find a_{new} such that $R_s(a_{new}) = m$.

We finally set

$$R_s(x) = \frac{w(x) P_{s-2}(x)}{w(a_{new}) P_{s-2}(a_{new})}. \tag{16}$$

ii) Computation of l_{new} (or d_{new}).

We have now to choose a new value of l. This gives a new value of $d = l/(1+a)$. Notice that this value must be bounded by the corresponding value for the optimal stability polynomials $\bar{l}$ (see (4) and (5)). We know that if a polynomial of order 2 and degree s alternates (with absolute value 1) on $s-1$ points of the stability interval, then it possesses the largest stability interval. We know also that $R_s(x)$ alternates asymptotically on $s-1$ points

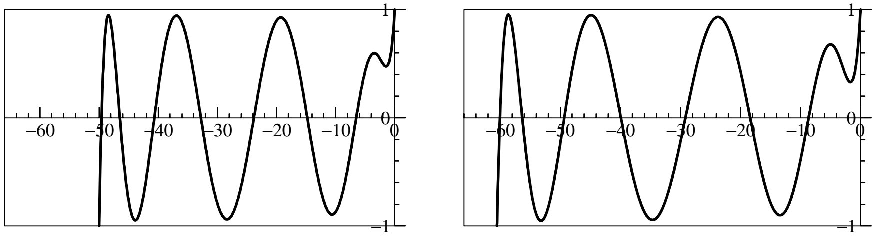

Fig. 5. Approximation polynomials (shifted) with $l_9 = 50$ (left), $l_9 = 60.5$ (right), $a = 0.99$, $\eta = 0.95$ (damping); see Fig. 3 for the polynomial of the same degree given after several iterations of the algorithm

of $[-1, 1]$ (see Sect. 2). We therefore try to choose l so that the local extrema of $R_s(x)$ are close to 1 (see Fig. 5). We define

$$\mu_i = \max_{x\in[\gamma_i,\gamma_{i+1}]} |R_s(x)| \quad i = 1, \ldots, s-2 \qquad \mu_{min} = \min_i \mu_i$$

(17)

$$l_{new} = l_{old} + \zeta(1 - \mu_{min}),$$

where γ_i $(i = 1, \ldots, s-2)$ are the real zeros of $R_s(x)$, $\gamma_{s-1} = a - \epsilon$ (ϵ as in (15)), and ζ is a positive parameter (for example $\zeta = 0.5$). If $l_{new} > \bar{l}$ or if $1 - \mu_{min} < tol$, where tol is a small positive parameter, then we define $l_{new} = l_{old}$.

In the end of this section we will give an asymptotic estimation of $\bar{l}$, the optimal stability interval (depending on the degree). Since we have necessarily that $l < \bar{l}$ ($\bar{l}$ is the optimal value for the real stability domain for a given degree s, see Sect. 2), we can use a fraction (for example $\frac{4}{5}$) of $\bar{l}$ as initial value for l.

We summarize now our algorithm. We suppose that initial values are given for a and l.

Algorithm.

1. Compute α_{new}, β_{new} which satisfy (14)
2. Compute a_{new} such that (15) is satisfied and compute l_{new} by (17)
3. Return to step 1 until $|a_{new} - a_{old}| < eps$ and $|l_{new} - l_{old}| < eps$, where eps is a small positive parameter

The outputs of this algorithm for a given degree are α, β, a and l. As explained in Sect. 2, in practice we will use a damping $\eta = 0.95$. Thus condition (15) should be replaced by $\max_{x\in[-1,a-\epsilon]} |R_s(x)| = \eta$, and condition (17) by $l_{new} = l_{old} + \zeta(\eta - \mu_{min})$.

It was observed by several authors that for order 2, the maximum of the stability interval for the optimal stability polynomials is given by

(18) $$\bar{l} = \bar{c}_2(s)s^2,$$

Table 1. The stability parameters of $R_s(x)$

Degree s	Stability region l_s	Value $c_2(s) = l_s/s^2$	Degree s	Stability region l_s	Value $c_2(s) = l_s/s^2$
5	19.063	0.762553	100	8098.4966	0.809850
10	79.5131	0.79513	250	50623.5000	0.809976
20	321.5129	0.803782	500	202498.5000	0.809994
50	2023.4864	0.809395	1000	809998.5000	0.809999

where $\bar{c}_2(s)$ is rapidly approaching the limit value 0.82 (without damping) (see [17, p. 365] and [6, p. 34]). With damping, this value must be smaller since the maximum of the stability interval decreases.

We have computed our approximation polynomials of order 2, for degree 3 up to degrees more than 1000 with damping $\eta = 0.95$. Table 1 gives, for some polynomials, the values of l_s and $c_2(s) = l_s/s^2$.

It can be observed that l_s behaves like $l_s \approx 0.81s^2$. For the stability polynomials used in van der Houwen-Sommeijer methods, the corresponding bound (with the same damping $\eta = 0.95$) behaves like $0.65s^2$ (see Fig. 6 for an example of such polynomials).

4 Results on existence and on the error constant of $R_s(x)$

In this section we will discuss the non-linear equations (9) (see Lemma 1 and Theorem 2). We will also show that the error constant of $R_s(x)$ is positive and we will give a bound for it (Theorem 3).

For $s \geq 3$ given, we denote by

$$P_{s-2}(x) = \prod_{i=1}^{s-2}(x - \gamma_i) \quad -1 < \gamma_1 < \ldots < \gamma_{s-2} < 1,$$

the orthogonal polynomial on $[-1, 1]$ of degree $s - 2 \geq 1$ associated with the weight function $w(x)^2/\sqrt{1 - x^2}$, where $w(x) = (x - (\alpha + i\beta))(x - (\alpha - i\beta))$. We set $\widetilde{R}_s(x) = w(x)P_{s-2}(x)$.

Troughout this section we will work with the following assumption (on the parameters α, β of the function $w(x)$):

$$\text{(H)} \quad \exists\, \xi_1, \xi_2 \quad \text{satisfying } \gamma_{s-2} < \xi_1 < \xi_2 < \alpha \quad \text{such that } \widetilde{R}'_s(\xi_i) = 0,$$

where γ_{s-2} is the largest real zero of $\widetilde{R}_s(x)$ and α the real part of the complex zeros of $w(x)$. It was shown in [1] that optimal stability polynomials of even order satisfy (H).

We will prove in Lemma 1 that there exist α and β such that the polynomial $\widetilde{R}_s(x)$ satisfies the assumption (H). Under the assumption (H) we will then show that for every α and β, with $-\delta \leq 1-\alpha \leq \delta$ and $0 \leq \beta \leq \delta$ (for some $\delta > 0$), there exist a, d such that the non-linear equations (9) are satisfied.

Lemma 1. *Let γ_{s-2} be the largest zero of $\widetilde{R}_s(x)$. There exists $\delta > 0$ such that for every α and β, with $-\delta \leq 1-\alpha \leq \delta$ and $0 \leq \beta \leq \delta$, there exist ξ_i $(i = 1, 2)$ satisfying $\gamma_{s-2} < \xi_1 < \xi_2 < \alpha$ such that*

$$\widetilde{R}'_s(\xi_i) = 0 \quad i = 1, 2. \tag{19}$$

Proof. Let $\widetilde{R}_s(x) = (x-(\alpha+i\beta))(x-(\alpha-i\beta))\prod_{i=1}^{s-2}(x-\gamma_i)$, with $-1 < \gamma_1 < \ldots < \gamma_{s-2} < 1$. For $x > \gamma_{s-2}$ define

$$g(x) = \frac{\widetilde{R}'_s(x)}{\prod_{i=1}^{s-2}(x-\gamma_i)} = 2(x-\alpha) + ((x-\alpha)^2+\beta^2)\sum_{i=1}^{s-2}\frac{1}{x-\gamma_i}.$$

Let $\alpha = 1$ and $\beta = 0$. We set $n = s-2$ and $\epsilon = (1-\gamma_n)/2$ $(\epsilon > 0)$. Then $g(1+\frac{\epsilon}{n}) > 0$ and we will show that $g(1-\frac{\epsilon}{n}) < 0$. Since γ_i depends continuously on α and β the same property holds in a neighborhood of 1, if $-\delta \leq 1-\alpha \leq \delta$ and $0 \leq \beta \leq \delta$ with some $\delta > 0$.

Since $g(x) > 0$ if x tends to γ_n (from the right), there exist ξ_1, ξ_2 satisfying $\gamma_n < \xi_1 < \xi_2 < \alpha$ such that $\widetilde{R}'_s(\xi_i) = 0 \quad i = 1, 2$.

The estimate $g(1-\frac{\epsilon}{n}) < 0$ folows from

$$\sum_{i=1}^{n}\frac{1}{(1-\frac{\epsilon}{n}-\gamma_i)} \leq \frac{n}{1-\frac{\epsilon}{n}-\gamma_n} = \frac{n}{2\epsilon-\frac{\epsilon}{n}} \leq \frac{n}{\epsilon}.$$

□

We now prove that there exist polynomials $R_s(x) = \frac{w(x)P_{s-2}(x)}{w(a)P_{s-2}(a)}$, as defined in (8), satisfying (9):

Theorem 2. *Suppose that $\widetilde{R}_s(x)$ satisfies (H) and $\beta \neq 0$, then there exist $a > \xi_2$ (where ξ_2 is the largest zero of $\widetilde{R}'_s(x)$) and d such that $R_s(x) = \frac{\widetilde{R}_s(x)}{\widetilde{R}_s(a)}$ satisfies*

$$R'_s(a,\alpha,\beta) = d, \quad R''_s(a,\alpha,\beta) = d^2. \tag{20}$$

Proof. Since $\beta \neq 0$ $\widetilde{R}_s(x)$ has $s-2$ real zeros and because of the assumption (H), $\widetilde{R}'_s(x)$ has $s-1$ real zeros, and its largest zero $\xi_2 > \gamma_{s-2}$, where γ_{s-2} is the largest zero of $\widetilde{R}_s(x)$. This implies that $\widetilde{R}''_s(x) > 0$ for $x \geq \xi_2$. Thus if we define $p(x) = (\widetilde{R}'_s(x))^2 - \widetilde{R}_s(x)\widetilde{R}''_s(x)$, we have $p(\xi_2) < 0$.

Since $p(x) = \mathcal{O}(x^{2s-3}) + sx^{2s-2}$, we have $p(x) > 0$ for x large. Hence, there exists $a > \xi_2$ such that $p(a) = 0$, i.e.

$$\left(\frac{\widetilde{R}'_s(a)}{\widetilde{R}_s(a)}\right)^2 = \frac{\widetilde{R}''_s(a)}{\widetilde{R}_s(a)}.$$

Table 2. Zeros of $w(x)$ and parameter a_s

Degree s	Zero α_s	Zero β_s	Parameter a_s
5	0.876008	0.138447	1.009632
10	0.968456	3.399721D-02	1.001578
20	0.992172	8.455313D-03	1.000433
50	0.998801	1.342920D-03	1.000114
100	0.999704	3.355449D-04	1.000032
250	0.999953	5.367668D-05	1.000006
500	0.999988	1.342131D-05	1.000001
1000	0.999997	3.354930D-06	1.0000003

Define $R_s(x) = \frac{\widetilde{R}_s(x)}{\widetilde{R}_s(a)}$ and $d = R_s'(a) > 0$; this gives formula (20). $\square$

In Table 2 we give the values of a_s, α_s, β_s corresponding to the polynomials of Table 1 (Sect. 3).

Lemma 1 and Theorem 2 show that for a given $s \geq 3$ and for every α and β, with $-\delta \leq 1 - \alpha \leq \delta$ and $0 \leq \beta \leq \delta$ (for some $\delta > 0$), there exist a, d such that the polynomial $R_s(x)$ as defined in (8) satisfies the nonlinear equations (9). Numerical computations show that the outputs of the algorithm of Sect. 3 are given asymptotically by $\alpha_s = 1 - \epsilon_s$ $\beta_s = \epsilon_s$ with $\epsilon_s \longrightarrow 0$ (see Table 2).

Let $R_s(x)$ be a polynomial given by Theorem 2. The next theorem deals with the error constant of

$$\hat{R}_s(z) = R_s(a + z/d) = 1 + z + \frac{z^2}{2!} + a_3 z^3 + \ldots$$

This polynomial is of second order, with an error constant given by

$$C = \frac{1}{3!} - a_3 \quad \text{where} \quad a_3 = \frac{R_s'''(a)}{3! d^3}, \tag{21}$$

where $d = R_s'(a)$. We will prove that $C \in (0, \frac{1}{6})$ (for all $s \geq 3$). Notice that for the parameter a given by Theorem 2, $a_3 > 0$.

Lemma 2. *Suppose that $Q(z)$ is a polynomial of order 2 (i.e. $Q(z) = 1 + z + \frac{z^2}{2!} + a_3 z^3 + \ldots$) such that $Q'(z)$ has only real zeros. Then the error constant $C = \frac{1}{3!} - a_3$ of $Q(z)$ is strictly positive.*

Proof. By hypothesis $Q'(z) = \prod_{i=1}^{s-1}(1 + \gamma_i z) = 1 + z + 3a_3 z^2 + \ldots$ where γ_i are reals. We have

$$s_1 = \sum_{i=1}^{s-1} \gamma_i = 1 \quad \text{and} \quad s_2 = \sum_{i<j} \gamma_i \gamma_j = 3a_3.$$

Since $s_1^2 - 2s_2 > 0$ we have $s_2 < \frac{s_1^2}{2} = \frac{1}{2}$, hence $a_3 < \frac{1}{6}$. □

We can now prove the following Theorem on the error constant of $\hat{R}_s(z)$:

Theorem 3. *Suppose* $R_s(x)$ *satisfies (H) and let* a *and* d *be given by Theorem 2. Then the error constant* C *of* $\hat{R}_s(z) = R_s(a + z/d)$ *satisfies* $C \in (0, \frac{1}{6})$.

Proof. Since $\hat{R}_s'(z)$ possesses only real zeros (because $R_s(x)$ satisfies (H)), we have by Lemma 2 that the error constant of $\hat{R}_s(z)$ is strictly positive. The estimate $C < 1/6$ follows from the fact that $a_3 > 0$. □

Remark 2. A similar, but more sharper bound than in Theorem 3, was shown for the error constants of optimal stability polynomials (for arbitrary orders and degrees).

5 Explicit formulas for orthogonal polynomials and recurrence relation

In the sequel we set $n \leq s-2$ ($s \geq 3$ given), and denote by $x_1 = \alpha + i\beta$, $x_2 = \alpha - i\beta$ the complex conjugate zeros of $w(x)$ ($\beta \neq 0$). Notice that all polynomials depend on s.

The aim of this section is to find a simple formula in order to compute the orthogonal polynomials $P_n(x)$ associated with the weight function $w^2(x)/\sqrt{(1-x^2)}$, and its recurrence coefficients. We will use a formula connecting two systems of orthogonal polynomials associated with different weight functions. The first such result was obtained by Christoffel [3].

Let us show that

(22)
$$w(x)^2 P_n(x) = C \underbrace{\begin{vmatrix} T_n(x_1) & T_n(x_2) & T_n'(x_1) & T_n'(x_2) & T_n(x) \\ T_{n+1}(x_1) & T_{n+1}(x_2) & T_{n+1}'(x_1) & T_{n+1}'(x_2) & T_{n+1}(x) \\ T_{n+2}(x_1) & T_{n+2}(x_2) & T_{n+2}'(x_1) & T_{n+2}'(x_2) & T_{n+2}(x) \\ T_{n+3}(x_1) & T_{n+3}(x_2) & T_{n+3}'(x_1) & T_{n+3}'(x_2) & T_{n+3}(x) \\ T_{n+4}(x_1) & T_{n+4}(x_2) & T_{n+4}'(x_1) & T_{n+4}'(x_2) & T_{n+4}(x) \end{vmatrix}}_{:= Q(x)}$$

where $T_n(x)$ are the Chebyshev polynomials of degree n and C is a constant depending on the normalization. Indeed, for $i = 1$ and 2,

$$Q(x_i) = 0 \text{ and } Q'(x_i) = 0 \Longrightarrow Q(x) = C_1(x - x_1)^2(x - x_2)^2 S_n(x)$$

where $S_n(x)$ is a polynomial of degree $\leq n$. We also have that $Q(x) = \sum_{i=0}^{4} b_i T_{n+i}(x)$ (definition of $Q(x)$). It remains to show that $S_n(x)$ is orthogonal with respect to $w(x)^2/\sqrt{1-x^2}$. Let $p(x)$ be a polynomial of degree $\leq n-1$ then

$$\int_{-1}^{1} p(x) S_n(x) \frac{w(x)^2}{\sqrt{1-x^2}} dx = \int_{-1}^{1} p(x) \sum_{i=0}^{4} T_{n+i}(x) \frac{1}{\sqrt{1-x^2}} dx = 0,$$

where the last equality is true because of the orthogonality property of the Chebyshev polynomials. It is not difficult to show (see [16, p. 29] for more details) that $S_n(x) \not\equiv 0$, thus of degree n, and the proof of formula (22) is complete.

In the sequel, we set again $z = (x-a)d$, in order to work in the interval $[-l, 0]$ (see (13)), and denote by $\hat{P}_n(z) = P_n(a + z/d)$ the shifted polynomial. It is well-known that orthogonal polynomials possess a three-term recurrence relation. Let us denote by

$$\hat{P}_n(z) = (\mu_n z - \nu_n)\hat{P}_{n-1}(z) - \kappa_n \hat{P}_{n-2}(z) \tag{23}$$

the recurrence formula of this system of orthogonal polynomials. The recurrence parameters μ_n, ν_n, κ_n can be determined by solving a linear system. We simply insert three different values for z into (23)

$$\mu_n r_i \hat{P}_{n-1}(r_i) - \nu_n \hat{P}_{n-1}(r_i) - \kappa_n \hat{P}_{n-2}(r_i) = \hat{P}_n(r_i) \quad i = 1, 2, 3 \tag{24}$$

such that

$$\begin{vmatrix} r_1 \hat{P}_{n-1}(r_1) & \hat{P}_{n-1}(r_1) & \hat{P}_{n-2}(r_1) \\ r_2 \hat{P}_{n-1}(r_2) & \hat{P}_{n-1}(r_2) & \hat{P}_{n-2}(r_2) \\ r_3 \hat{P}_{n-1}(r_3) & \hat{P}_{n-1}(r_3) & \hat{P}_{n-2}(r_3) \end{vmatrix} \neq 0. \tag{25}$$

Then (24) consists in a linear system which determines uniquely μ_n, ν_n and κ_n.

6 Construction of the numerical method and ROCK2

6.1 Definition of the method

In this section, we want to construct a Runge-Kutta method which possesses the polynomials $\hat{R}_s(z) = \hat{w}(z)\hat{P}_{s-2}(z)$ (constructed in Sect. 3) as stability polynomials.

Following the idea of [8], the three-term recurrence relation (23) can be naturally used to define the internal stages of the numerical method

$$\begin{aligned} g_0 &:= y_0 \\ g_1 &:= y_0 + h\mu_1 f(g_0) \\ g_j &:= h\mu_j f(g_{j-1}) - \nu_j g_{j-1} - \kappa_j g_{j-2} \quad j = 2, \ldots, s-2. \end{aligned} \tag{26}$$

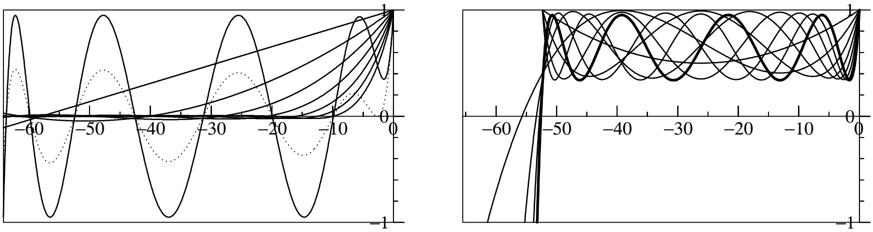

Fig. 6. $\hat{R}_9(z)$ and the stability polynomial of the method $g_9^\star$ in dotted line (left), $R(z) = a_9 + b_9 T_9(w_0 + w_1 z)$ (right); in both figures the stability polynomials of all internal stages are drawn

Then, the quadratic factor $\hat{w}(z) = 1 + 2\sigma z + \tau z^2$ is represented by a two-stage "finishing procedure" similar as in [9]

$$\begin{aligned} g_{s-1} &:= g_{s-2} + h\sigma f(g_{s-2}) \\ g_s^\star &:= g_{s-1} + h\sigma f(g_{s-1}) \\ g_s &:= g_s^\star - h\sigma(1 - \tfrac{\tau}{\sigma^2})(f(g_{s-1}) - f(g_{s-2})). \end{aligned} \tag{27}$$

For $y' = \lambda y$ we obtain

$$\begin{aligned} g_j &= \hat{P}_j(z) g_0 \qquad j = 0, \ldots, s-2 \\ g_s &= \hat{w}(z) g_{s-2} \end{aligned} \tag{28}$$

where $z = h\lambda$. Hence,

$$g_s = \hat{R}_s(z) g_0. \tag{29}$$

In Fig. 6 (left), we sketched an example (for $s = 9$) of $\hat{R}_s(z)$ and $\hat{P}_j(z)$, the stability functions of the internal stages. For the same degree we sketched the van der Houwen-Sommeijer stability polynomial $R(z) = a_9 + b_9 T_9(w_0 + w_1 z)$, and its internal stability polynomials (Fig. 6 right).

6.2 Error estimate

For the error estimate, $g_s^\star$ can be used as an embedded method. The stability polynomial of this method is

$$R_s^\star(z) = (1 + 2\sigma z + \sigma^2 z^2)\hat{P}_{s-2}(z) = w^\star(z)\hat{P}_{s-2}(z). \tag{30}$$

Since $\hat{R}_s(z) = (1 + 2\sigma z + \tau z^2)\hat{P}_{s-2}(z) = \hat{w}(z)\hat{P}_{s-2}(z)$ is of order 2, $R_s^\star(z)$ is of order 1.

Recall that $\hat{w}(z) > 0\, \forall z$ and that $|\hat{R}_s(z)| \le \eta$ for $z \in [-l_s, -\epsilon]$, where ϵ is a small positive number (see Sect. 3 and 4). Let us show that the absolute value of $R_s^\star(z)$ is bounded by η in the same interval as $\hat{R}_s(z)$ (see Fig. 6 left).

Lemma 3. *Suppose that* $|\hat{R}_s(z)| \leq \eta$ *for* $z \in [-l_s, -\epsilon]$ *and* $\hat{w}(z) > 0\, \forall z$. *Then the polynomial* $R_s^\star(z)$ *as defined in (30) satisfies*

$$|R_s^\star(z)| < \eta\, \forall z \in (-l_s, -\epsilon).$$

Proof. A simple computation shows that $w^\star(z) \geq 0\, \forall z$. Now, since $\hat{w}(z) > 0\, \forall z$, we have that $\tau > \sigma^2$, hence $\hat{w}(z) - w^\star(z) = (\tau - \sigma^2)z^2 > 0$. This yields

$$|R_s^\star(z)| = |w^\star(z)||\hat{P}_{s-2}(z)| \leq |\hat{w}(z)||\hat{P}_{s-2}(z)| \leq \eta\, \forall z \in [-l_s, -\epsilon].$$

We conclude the proof by noting that the first inequality is an equality only if $\hat{P}_{s-2}(z) = 0$. □

As a measure of the error after one step we take

$$err = \|g_s - g_s^\star\|. \tag{31}$$

For the step size selection, we used the " step size control with memory " introduced by Watts [18] and Gustafsson [4]

$$h_{\text{new}} = \text{fac} \cdot h_n \Big(\frac{1}{\text{err}_{n+1}}\Big)^{1/2} \frac{h_n}{h_{n-1}} \Big(\frac{\text{err}_n}{\text{err}_{n+1}}\Big)^{1/2}, \tag{32}$$

in order to allow the step size to decrease more than a factor *fac* without step rejections. The conventional prediction is obtained by deleting the terms after the first brackets in (32). As advised in [6, p.125] we used for h_{new} the minimum of the step sizes proposed by (32) and the conventional strategy. This latter strategy is also used after a step rejection.

6.3 Step size and stage number selection, spectral radius estimation

We showed in Theorem 3 that the error constants of $\hat{R}_s(z)$ are all in the interval $(0, \frac{1}{6})$. It was found numerically that the error constants of $\hat{R}_s(z)$, rapidly decrease to a limit value (this was discussed in [1] for optimal stability polynomials). It means that the error constants are almost independent of the number of stages of the numerical method. Thus, at each step, our code chooses first the new stepsize in order to control the local error, then it selects the number of stages in order to satisfy the stability condition

$$h\rho\left(\frac{\partial f}{\partial y}(y)\right) \leq 0.81 s^2, \tag{33}$$

where ρ is the spectral radius of the Jacobian matrix of the ODE.

We also implemented an automatic computation of this spectral radius. For that we used a non-linear power method which is a slight modification of the algorithm proposed by B.P. Sommeijer, L.F. Shampine and J.G. Verwer (see [15]). The user has still the choice to give an estimation of the spectral radius by himself.

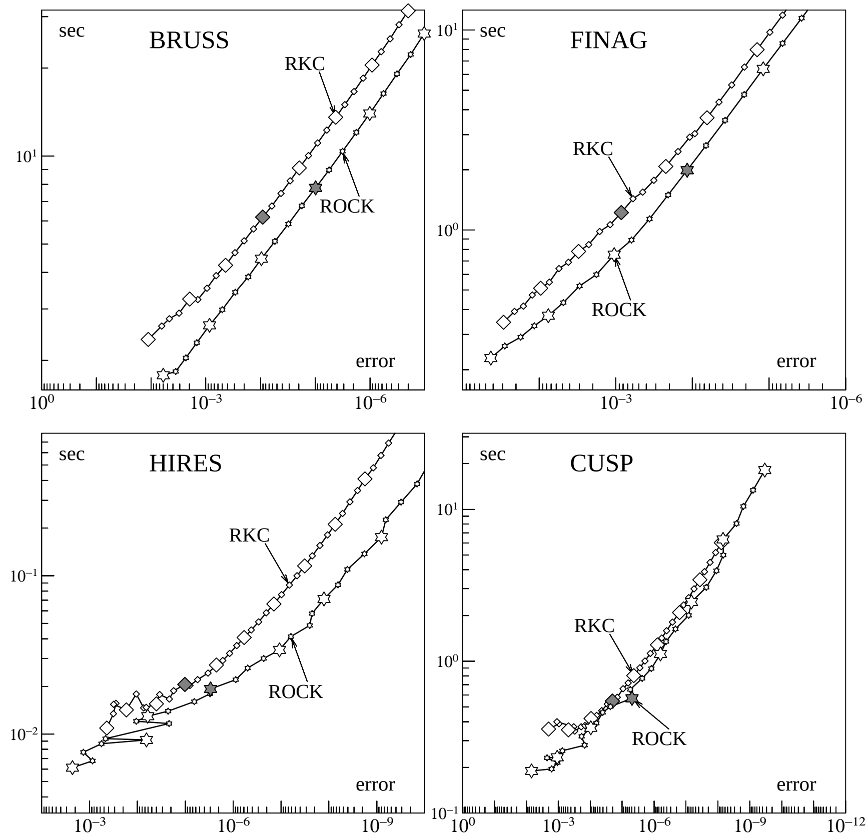

Fig. 7. Comparison of Chebyshev codes

7 Numerical experiments

We conclude this paper by presenting some results of numerical experiments. The numerical methods described in Sect. 6 have been incorporated in an experimental code called ROCK2. The performance of this code has been compared with the latest version of RKC [15]. Both codes have second order.

We chose the following stiff problems from [6] (first and second editions):

1. BRUSS: The Brusselator, chemical reaction (diffusion) converted into ODE's by the method of lines. This is a system of 1000 equations with the largest eigenvalues close to -20000. This problem is very stiff.
2. FINAG: The FitzHug and Nagumo nerve conduction equation, converted into ODE's by the method of lines. This is a system of 400 equations.
3. HIRES: A chemical reaction proposed by Schäfer, which is given by 8 equations.

4. CUSP: The Zeeman's "cusp catastrophe" model ($-\epsilon\dot{y} = y^3 + ay + b$) for the nerve impulse mechanism, combined with the van der Pol oscillator, converted into ODE's by the method of lines. This is a system of 96 equations.

All parameters and outputs for these problems are chosen as in [6] (first and second editions). We solved these problems by varying the value of the tolerance:

$$Tol = 10^{-2-m/4} \quad m = 1, 2, 3, \dots .$$

The results are represented in Fig. 7 in logarithmic scales (in the abscissa the accuracy, in the ordinate the computed time in seconds). The integer exponent tolerances $10^{-2}, 10^{-3}, \dots$ are displayed as enlarged symbols. The tolerance 10^{-5} is distinguished by its gray colour. For all problems we took scalar tolerances $atol = rtol = tol$ and we provide for both codes an estimation of the spectral radius of the Jacobian matrix. We see on Fig. 7 that ROCK2 behaves well and that it also preserves nicely the tolerance proportionality.

Source code for ROCK2 and some examples are available on the Internet at the address
http://www.unige.ch/math/folks/hairer/software.html
Experiences with this code are welcome.

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