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Explicit Stabilized Runge-Kutta Methods

Synonyms

Chebyshev methods, Runge-Kutta-Chebyshev methods

Definition

Explicit stabilized Runge-Kutta (RK) methods are explicit one-step methods with extended stability domains along the negative real axis. These methods are intended for large systems of ordinary differential equations originating mainly from semi-discretization in space of parabolic or hyperbolic-parabolic equations. The methods do not need the solution of large linear systems at each step size (as e.g., implicit methods). At the same time due to their extended stability domains along the negative real axis, they have less severe step size restriction than classical explicit methods when solving stiff problems.

Overview

For solving time-dependent partial differential equations (PDEs) a widely-used approach is to first discretize the space variables to obtain a system of ordinary differential equations (ODEs) of the form

$$y' = f(t, y), \quad y(t_0) = y_0, \tag{1}$$

where $y, y_0 \in \mathbb{R}^n,\ t \geq 0$ and $f(t, y)$ has value in $\mathbb{R}^n$. The class of problems of interest for explicit stabilized RK methods are problems for which the eigenvalues of the Jacobian matrix $\frac{\partial f}{\partial y}$ are known to lie in a long narrow strip along the negative real axis. This situation typically arises when discretizing parabolic equations or hyperbolic-parabolic equations such as advection-diffusion-reaction equations (with dominating diffusion).

Solving large stiff systems

ODEs arising from semi-discretization of parabolic or hyperbolic-parabolic PDEs are usually large, as the dimension n of the system is proportional to $1/\Delta x$, where Δx is the spatial discretization length. Classical explicit one-step methods, as for example the explicit Euler method

$$y_{k+1} = y_k + \Delta t f(t_k, y_k),$$

must satisfy the stringent so-called Courant-Friedrich-Lewy (CFL) condition [11] $\Delta t \leq C(\Delta x)^2$ in order for the numerical solution $\{y_k\}_{k\geq 0}$ to remain bounded. The above CFL condition leads to a numerical method with a huge number of steps, with step size usually much smaller than required for accuracy reasons. Classes of implicit one-step methods such as the implicit Euler method

$$y_{k+1} = y_k + \Delta t f(t_{k+1}, y_{k+1})$$

are known to be stable for ODEs arising from the semi-discretization of hyperbolic-parabolic PDEs. But the good stability properties of implicit methods are obtained

at the cost of solving nonlinear equations at each step. Although efficient in many situations, this approach can be expensive especially for large systems.

Linear stability analysis of one-step methods

The linear stability analysis for one-step methods is based on the following transformations. By linearizing the ODE (1) a system $w'(t) = A(t)w(t)$ is obtained, where $A(t)$ represents the Jacobian matrix of the original system. Next, freezing the time parameter in $A(t)$ and finally transforming the linear equation into diagonal or Jordan form one is lead to consider the Dahlquist test equation [12]

$$y' = \lambda y, \ \lambda \in \mathbb{C}. \tag{2}$$

Applying an RK to (2) gives $y_k = R(z)^k y_0$, where $R(z)$ is a rational function and $z = \Delta t\lambda$. This rational function is called the stability function of the method. As an example, for the explicit or implicit Euler method, we have

$$y_k = (1+z)y_{k-1} = (1+z)^k y_0, \tag{3}$$

$$y_k = \left(\frac{1}{1-z}\right)^k y_0, \tag{4}$$

respectively. The condition $|R(z)| \leq 1$ ensures that $\{y_k\}_{k\geq 0}$ remains bounded and leads to the definition of the stability domain of a numerical method

$$\mathcal{S} := \{z \in \mathbb{C}; |R(z)| \leq 1\}. \tag{5}$$

For example, the stability domain of the explicit Euler method is a disk of radius 1 in the complex plane centered in -1, while the stability domain of the implicit Euler method is the complementary set of a disk of radius 1 centered in 1.

As the Jacobian of the system of ODEs obtained from spatial discretization of parabolic problems has eigenvalues distributed along the negative real axis with a spectral radius growing proportional to $1/(\Delta x)^2$ [11], the stability condition for the

explicit Euler method reads $\Delta t \leq C(\Delta x)^2$. The implicit Euler is unconditionally stable for this problem, but this comes at the price of solving large linear systems of size proportional to $(1/(\Delta x))^d$ (d is the spatial dimension) at each step size. Explicit stabilized Runge-Kutta methods are a compromise between the two aforementioned methods in the following sense: the explicitness of the methods allows to avoid to solve (possibly large) linear systems at each step size, the extended stability domains along the negative real axis allow to avoid the usual step size restriction encountered with classical explicit methods. Such methods have been pioneered by Saul'ev [30], Guillou and Lago [15] Gentsch and Schlüter [14]. Recent developments include the methods based on recurrence relation [34; 35], the methods based on composition [24; 20; 22; 27; 33] and the methods combining recurrence relation and composition [7; 3]. We also mention the extension of these methods to stiff stochastic problems [5; 6].

Basic Methodology

Explicit stabilized Runge-Kutta methods are constructed in two steps. First, stability polynomials bounded in a long strip around the negative real axis are constructed. Second, numerical methods with such favorable stability functions are constructed.

Optimal stability polynomials on the negative real axis

The basic idea Saul'ev [30], Guillou and Lago [15] Gentsch and Schlüter [14] to overcome the step size restriction for classical explicit methods is to consider a composition of (classical) explicit methods with a super step size. Consider for example a sequence of explicit Euler methods $g_{h_1}, \ldots, g_{h_s}$ with a corresponding sequence of step sizes $h_1, \ldots, h_s$ and define a one-step method as the composition

$$y_1 = (g_{h_s} \circ \ldots \circ g_{h_1})(y_0), \tag{6}$$

with step size $\Delta t = h_1 + \ldots + h_s$. Applied to (2), this methods yields the stability function $R_s(z) = \prod_{i=1}^{s}(1 + h_i z)$. Next, given s, optimize the sequence $\{h_i\}_{i=1}^{s}$, so that

$$R_s(z) = 1 + z + \mathcal{O}(\Delta z^2), \quad |R_s(z)| \leq 1 \ \text{ for } z \in [-l_s, 0], \tag{7}$$

with $l_s > 0$ as large as possible. The first condition is necessary for Method (6) to have first order accuracy, the second condition ensures an optimal stability region along the negative real axis. Problem (7) can be reformulated in the following way: find $\alpha_2, \ldots, \alpha_s \in \mathbb{R}$ such that $R_s(z) = 1 + z + \sum_{i=2}^{s} \alpha_i z^i$ satisfies $|R_s(z)| \leq 1 \ \text{ for } z \in [-l_s, 0]$ with $l_s > 0$ as large as possible. We recall that a Runge-Kutta method is said to be accurate with order p if and only if

$$\|y(t_0 + \Delta t) - y_1\| = \mathcal{O}\left((\Delta t)^{p+1}\right). \tag{8}$$

Condition (8) implies that the stability function of a Runge-Kutta method of order p satisfies

$$R_s(z) = 1 + z + \frac{z^2}{2!} + \ldots + \frac{z^p}{p!} + \mathcal{O}\left(z^{p+1}\right). \tag{9}$$

We notice that for $p \leq 2$, (9) implies (8) [17, Sect. II.1].

As noticed in [26; 37; 13; 15], the solution of problem (7) is given by shifted Chebyshev polynomials $R_s(z) = T_s(1 + z/s^2)$ where $T_s(\cdot)$, the Chebyshev polynomial of degree s, is given by

$$T_0(z) = 1, \quad T_1(z) = z, \quad T_j(z) = 2zT_{j-1}(z) - T_{j-2}(z), \ j \geq 2. \tag{10}$$

The equi-oscillation property of $R_s(x)$, i.e., the existence of s points $0 > x_1 > x_2 > \ldots > x_s$ such that $|R_s(x_i)| = 1$ for $i = 1, \ldots, s$ and $R_s(x_{i+1}) = -R_s(x_i)$ for $i = 1, \ldots, s-1$, is used to show that $R_s(z) = T_s(1 + z/s^2)$ is indeed the solution of Problem (7). We notice that these properties are inherited from corresponding properties of the Chebyshev polynomials. As a consequence, the optimal sequence of $\{h_i\}_{i=1}^{s}$ is given by $h_i = -1/z_i$, where z_i are the zeros of $R_s(z)$ and we have $|R_s(z)| \leq 1 \ \text{ for } z \in [-l_s, 0]$

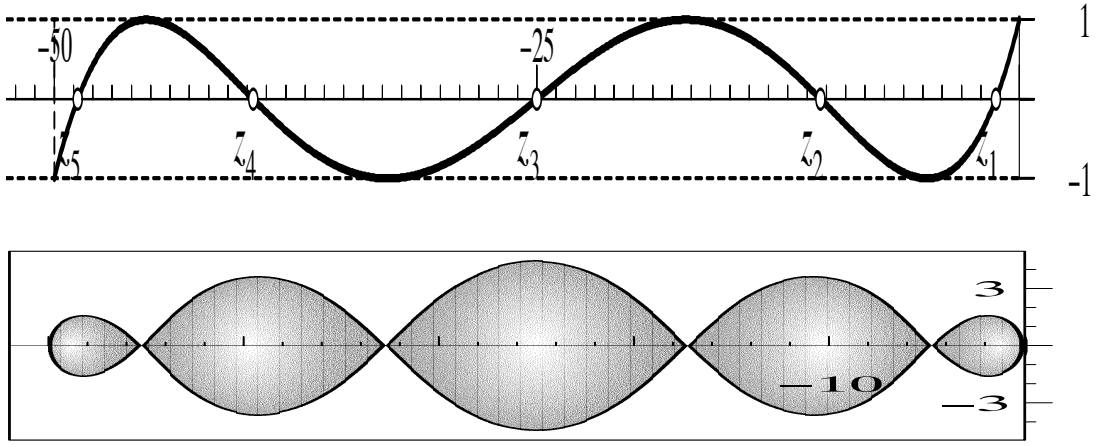

Fig. 1. Shifted Chebyshev polynomial of degree 5, $R_5(z),\ z \in \mathbb{R}$ (upper Figure). Stability domain of $\mathcal{S} := \{z \in \mathbb{C}; |R_5(z)| \leq 1\}$ (lower Figure).

with $l_s = 2s^2$ (see Figure 1). The fact that the maximal stability domain on the negative real axis increases quadratically with the number of stages s is crucial to the success of stabilized Runge-Kutta methods.

Complexity and cost reduction

Assume that the accuracy requirement dictates a step size of Δt and that the Jacobian of Problem (1) has eigenvalues close to the real negative axis with a spectral radius given by Λ (possibly large). For a classical explicit Runge-Kutta method the stability constraint forces to take a step size $h \simeq C/\Lambda$ which leads to $N = \Delta t\Lambda/C$ function evaluations per step size Δt. For example, for the explicit Euler method, this cost reads $N = \Delta t\Lambda/2$. For an explicit stabilized Runge-Kutta method with a stability interval along the negative real axis given by $l_s = C \cdot s^2$ we choose $\Delta t\Lambda = C \cdot s^2$ which gives $s = \sqrt{\Delta t\Lambda/C}$. For the first order method stabilized Runge-Kutta method, with a stability function given by $R_s(z) = T_s(1 + z/s^2)$, we obtain $s = \sqrt{\Delta t\Lambda/2}$, the square root of the cost of the explicit Euler method.

Construction of explicit stabilized Runge-Kutta methods

Given a stability polynomial with optimal stability around the negative real axis, the goal is now to construct corresponding Runge-Kutta methods. There are two main strategies to realize such Runge-Kutta methods. The first idea (and also the oldest) is, as already seen, by composition of Euler steps. The second idea exploits the three-term recurrence relation of the Chebyshev polynomials. For simplicity we consider autonomous ODEs, e.g., $y' = f(y)$, but emphasize that the methods described below can be applied to general ODEs by appending the differential equation $t' = 1$ to the autonomous differential equation.

Methods by composition

This approach first proposed by Saul'ev [30] and Guillou & Lago [15] is based on a composition of Euler steps (6)

$$g_i = g_{i-1} + h_i f(g_{i-1}),\ i = 1, \ldots, s, \quad y_1 = g_s, \tag{11}$$

where $g_0 = y_0$, $h_i = \gamma_i \Delta t$, $\gamma_i = -1/z_i$ and z_i are the zeros of the shifted Chebyshev polynomials. The g_i are called the internal stages of the method. Without special ordering of the step sizes, internal instabilities such as round-off error can propagate within a single integration step Δt in such a way that makes the numerical method useless [18] (recall that we aim at using a large number of internal stages, e.g., $s \geq 100$). A strategy to improve the internal stability of the method (11) based on a combination of large and small Euler steps has been proposed in [14].

Methods by recurrence

First proposed by van der Houwen and Sommeijer [34], this approach uses the three-term recurrence relation (10) of the Chebyshev polynomials to define a numerical method given by

$$g_1 = g_0 + \frac{\Delta t}{s^2} f(g_0), \quad g_i = \frac{2\Delta t}{s^2} f(g_{i-1}) + 2g_{i-1} - g_{i-2},\ i = 2, \ldots, s, \quad y_1 = g_s, \quad (12)$$

where $g_0 = y_0$. One verifies that applied to the test problem $y' = \lambda y$, this method gives for the internal stages

$$g_i = T_i(1 + \Delta t\lambda/m^2) y_0,\ i = 0, \ldots, s, \quad (13)$$

and produces after one step $y_1 = g_s = T_s(1 + x/s^2) y_0$. Propagation of rounding errors within a single step is reasonable for this method even for large values of s such as used in practical computation [34].

Damping

It was first observed by Guillou & Lago [15] that one should replace the stability requirement $|R_s(z)| \leq 1,\ z \in [-l_s, 0]$ by $|R_s(z)| \leq \eta < 1,\ z \in [-l_{s,\eta}, -\delta_\eta]$, where δ_η a small positive parameter depending on η. Indeed, for the points $x_i \in \mathbb{R}^-$ where $R(x_i) = T_s(1 + x_i/s^2) = \pm 1$, the stability domain has zero width (see Figure 2). If one sets

$$R_s(z) = \frac{1}{T_s(\omega_0)} T_s(\omega_0 + \omega_1 z), \quad \omega_0 = 1 + \frac{\eta}{s^2}, \quad \omega_1 = \frac{T_s(\omega_0)}{T_s'(\omega_0)}, \quad (14)$$

then the polynomials (14) oscillate approximately between $-1 + \eta$ and $1 - \eta$ (this property is called "damping"). The stability domain along the negative real axis is a bit shorter, but the damping ensures that a strip around the negative real axis is included in the stability domain (see Figure 2). Damping techniques also allow to consider hyperbolic-parabolic problems. By increasing the value of η, a larger strip around the negative real axis can be included in the stability domains. This has been considered for explicit stabilized Runge-Kutta methods in [33; 36]. Recently damping techniques have also been used to extend stabilized Runge-Kutta methods for stiff stochastic problems [4; 6].

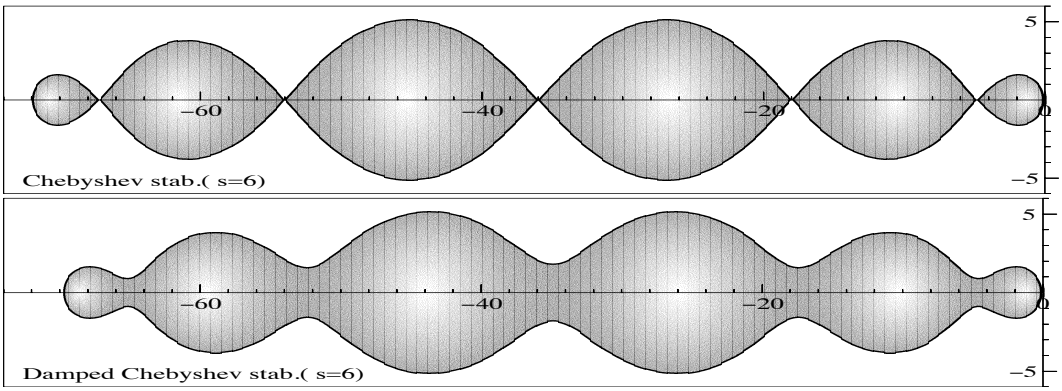

Fig. 2. Stability domain for shifted Chebyshev polynomials of degree 6. Undamped polynomial (upper Figure) and damped polynomial with $\eta = 0.95$ (lower Figure).

Higher-order methods

Both problems, constructing optimal stability polynomials and deriving related Runge-Kutta methods are considerably more difficult for higher order. First, we have to find a polynomial of order p, i.e. $R(z) = 1 + z + \ldots + \frac{z^p}{p!} + \mathcal{O}(z^{p+1})$, and degree s such that

$$R_s(z) = 1 + z + \ldots + \frac{z^p}{p!} + \alpha_{p+1} z^{p+1} + \ldots + \alpha_s z^s, \quad |R_s(z)| \leq 1 \text{ for } z \in [-l_s^p, 0], \quad (15)$$

with l_s^p as large as possible. The existence and uniqueness of such polynomials with maximal real negative stability interval, called *optimal stability polynomials*, for arbitrary values of p and s has been proved by Riha [29]. No elementary analytical solutions are known for these polynomials for $p > 1$. Lebedev [23] found analytic expressions for second order optimal polynomials in terms of elliptic functions related to Zolotarev polynomials. Abdulle [1] gave a classification of the number of complex and reals zeros of the optimal stability polynomials as well as bounds for the error constant $C_s^p = 1/(p+1)! - \alpha_{p+1}$. In particular, optimal stability polynomials of order p have exactly p complex zeros for even values of p and exactly $p-1$ complex zeros for odd values of p. In practice such polynomials are approximated numerically [2; 19; 18; 21; 25; 28]. As for first order optimal stability polynomials, higher order

optimal stability polynomials enjoy a quadratic growth (with s) of the stability region along the negative real axis

$$l_s^p \simeq c_p \cdot s^2, \quad c_2 = 0.82,\ c_3 = 0.49,\ c_4 = 0.34. \tag{16}$$

Approximations of l_s^p up to order $p = 11$ can be found in [2].

Several strategies for approximating the optimal stability polynomials have been proposed. The three main algorithms correspond to the the DUMKA methods (optimal polynomials without recurrence relation), the Runge-Kutta-Chebyshev (RKC) methods (non optimal polynomials with recurrence relation) and the orthogonal Runge-Kutta-Chebyshev (ROCK) methods (near optimal polynomials with recurrence relation). The construction of explicit stabilized Runge-Kutta-Chebyshev methods is then based on composition (DUMKA type methods), recurrence formulas (RKC type methods) and a combination of composition and recurrence formulas (ROCK type methods). An additional difficulty for methods of order $p > 2$ is that the structure of the stability functions $1 + z + \ldots + \frac{z^p}{p!} + \mathcal{O}(z^{p+1})$ guaranties the order p only for linear problems. Additional order conditions have to be built in the method to have order p also for nonlinear problems. Only DUMKA and ROCK type methods exist for $p > 2$.

DUMKA methods

DUMKA methods are based on the zeros of the optimal stability polynomials, computed through an iterative procedure [21]. Then, as suggested by Lebedev in [20; 22], one groups the zeros by pairs (if a zero is complex it should be grouped with its complex conjugate), considers quadratic polynomials of the form $(1-\frac{z}{z_i})(1-\frac{z}{z_j}) = 1+2\alpha_i z+\beta_i z^2$ and represents them as

$$\begin{aligned} g_i &:= g_{i-1} + \Delta t \alpha_i f(g_{i-1}) \\ g^*_{i+1} &:= g_i + \Delta t \alpha_i f(g_i) \\ g_{i+1} &:= g^*_{i+1} - \Delta t(\alpha_i - \tfrac{\beta_i}{\alpha_i})(f(g_i) - f(g_{i-1})). \end{aligned} \tag{17}$$

One step of the method consists of a collection of two-stage schemes (17). The above procedure allows to represent complex zeros and almost halves the largest Euler step. As for first order explicit stabilized RK methods, special ordering of the zeros is needed to ensure internal stability. This ordering is done "experimentally" and depends on the degree of the stability polynomial [24]. An extension for higher order has been proposed by Medovikov [27] (order 3 and 4).

RKC methods

RKC methods rely on introducing a correction to the first order shifted Chebyshev polynomial to allow for second order polynomials. These polynomials, introduced by Bakker [8] are defined by

$$R_s(z) = a_s + b_s T_s(w_0 + w_1 z), \tag{18}$$

where

$$a_s = 1 - b_s T_s(w_0), \quad b_s = \frac{T''_s(w_0)}{(T'_s(w_0))^2}, \quad w_1 = \frac{T'_s(w_0)}{T''_s(w_0)}, \quad w_0 = 1 + \frac{\epsilon}{s^2}, \quad \epsilon \simeq 0.15.$$

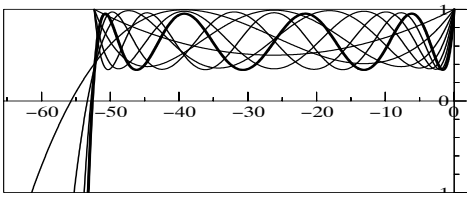

Fig. 3. Second order RKC polynomial of degree 9 (bold line). All internal stages are drawn (thin lines).

Polynomials (18) remain bounded by $\eta \simeq 1 - \epsilon/3$ on their stability interval (except for a small interval near the origin). The stability intervals are approximately given by $-0.65 \cdot s^2$ and cover about 80% of the stability intervals of the optimal second order stability polynomials. For the internal stages, the polynomials

$$R_j(z) = a_j + b_j T_j(w_0 + w_1 z),\ j = 0, \ldots, s-1,$$

can be used. To have consistent internal stages one must have $R_j(0) = 1$ and thus $a_j = 1 - b_j T_j(w_0)$. It remains to determine $b_0, \ldots, b_{s-1}$. If one requires the polynomials $R_j(z)$ for $j \geq 2$ to be of second order at nodes $t_0 + c_i \Delta t$ in the interval $[t_0, t_0 + \Delta t]$, i.e., $R_j(0) = 1,\ (R_j'(0))^2 = R_j''(0)$, then $R_j(z) = 1 + b_j(T_j(w_0 + w_1 z) - T_j(w_0))$, with $b_j = \frac{T_j''(w_0)}{(T_j'(w_0))^2}$ for $j \geq 2$. The parameters b_0, b_1 are free parameters (only first order is possible for $R_1(z)$ and $R_0(z)$ is constant) and the values $b_0 = b_1 = b_2$ are suggested in [31]. Using the recurrence formula of the Chebyshev polynomials the RKC method as defined by van der Houwen and Sommeijer [34] reads

$$\begin{aligned} g_1 &= g_0 + b_1 w_1 \Delta t f(g_0) \\ g_i &= g_0 + \mu_i \Delta t (f(g_{i-1}) - a_{i-1} f(g_0)) + \nu_i (g_{i-1} - y_0) + \kappa_i (g_{i-2} - y_0),\ i = 2, \ldots, s \\ y_1 &= g_s, \end{aligned} \tag{19}$$

where

$$\mu_i = \frac{2 b_i w_1}{b_{i-1}}, \quad \nu_i = \frac{2 b_i w_0}{b_{i-1}}, \quad \kappa_i = \frac{-b_i}{b_{i-2}},\ i = 2, \ldots, s.$$

ROCK methods

The orthogonal Runge-Kutta Chebyshev methods (ROCK) [2; 3; 7] are obtained through a combination of the approaches of Lebedev (DUMKA) and van der Houwen and Sommeijer (RKC). These methods possess nearly optimal stability polynomials, are build on recurrence relation and have been obtained for order $p = 2, 4$. As the

optimal stability polynomials of even order have exactly p complex zeros [1], the idea is to search, for a given p, an approximation of (15) of the form

$$R_s(x) = w_p(x) P_{s-p}(x), \tag{20}$$

where $P_{s-p}(x)$ is a member of a family of polynomials $\{P_j(x)\}_{j\geq 0}$ orthogonal with respect to the weight function $\frac{w_p(x)^2}{\sqrt{1-x^2}}$. The function $w_p(x)$ is a positive polynomial of degree p. By an iterative process one constructs $w_p(x)$ such that

- the zeros of $w_p(x)$ are close to the p complex zeros of (15);
- the polynomial $R_s(x)$ satisfies the $p-$th order condition, i.e.,

$$R_s(x) = w_p(x) P_{s-p}(x) = 1 + z + \ldots + \frac{z^p}{p!} + \mathcal{O}(z^{p+1}).$$

The theoretical foundation of such an approximation is a theorem of Bernstein [9], which generalizes the property of minimality and orthogonality of Chebyshev polynomials to more general weight functions. For $p = 2, 4$ such families of polynomials (depending on s) can be constructed with nearly optimal stability domains. Thanks to the recurrence relation of the orthogonal polynomials $\{P_j(x)\}_{j\geq 0}$, a method based on recurrence formula can be constructed.

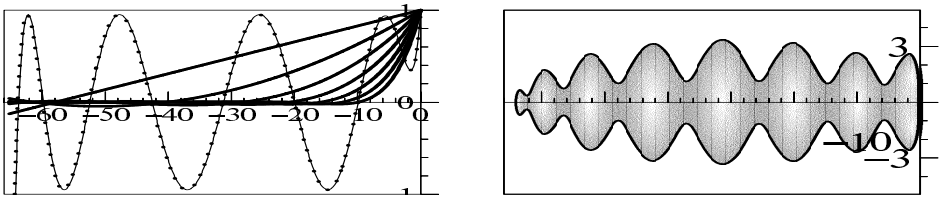

Fig. 4. Second order ROCK polynomial of degree 9 (thin line) with damping $\eta = 0.95$. All internal stages are drawn (bold lines). The optimal stability polynomial is displayed in dotted line.

Second order ROCK2 methods. We consider the polynomials (20) for $p = 2$. The three-term recurrence formula associated with the polynomials $\{P_j(x)\}_{j\geq 0}$

$$P_j(x) = (\alpha_j x - \beta_j) P_{j-1}(x) - \gamma_j P_{j-2}(x),$$

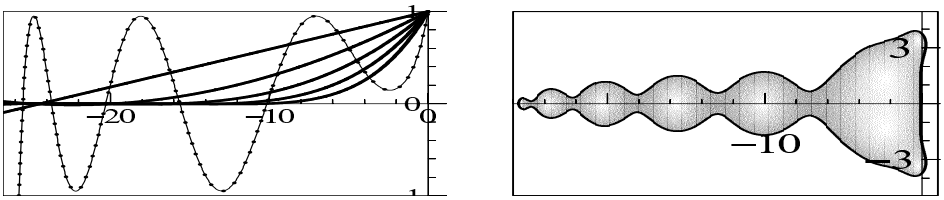

Fig. 5. Fourth order ROCK polynomial of degree 9 (thin line) with damping $\eta = 0.95$. All internal stages are drawn (bold lines). The optimal stability polynomial is displayed in dotted line.

is used to define the internal stages of the method

$$g_1 = y_0 + \alpha_1 \Delta f(g_0), \quad g_i = y_0 + \alpha_i \Delta f(g_{i-1}) - \beta_i g_{i-1} - \gamma_i g_{i-2}, \ i = 2, \ldots, s-2. \quad (21)$$

Then, the quadratic factor $w_2(z) = 1+2\sigma z+\tau z^2$ is represented by a two-stage "finishing procedure" similarly as in [22]

$$\begin{aligned} g_{s-1} &:= g_{s-2} + h\sigma f(g_{s-2}) \\ g_s^\star &:= g_{s-1} + h\sigma f(g_{s-1}) \\ g_s &:= g_s^\star - h\sigma(1 - \tfrac{\tau}{\sigma^2})\big(f(g_{s-1}) - f(g_{s-2})\big). \end{aligned} \quad (22)$$

For $y' = \lambda y$ we obtain

$$\begin{aligned} g_j &= P_j(z) g_0 \qquad\qquad j = 0, \ldots, s-2 \\ g_s &= w_2(z) P_{s-2}(z) = R_s(z) y_0, \end{aligned} \quad (23)$$

where $z = h\lambda$.

Fourth order ROCK4 methods. We consider the polynomials (20) for $p = 4$. Similarly to (21), we use the three-term recurrence formula associated with the polynomials $\{P_j(x)\}_{j\geq 0}$ to define the internal stages of the method $g_1, \ldots, g_{s-4}$.

For the finishing procedure, simply implementing successively two steps like (22) will only guarantee the method to be of fourth order for linear problems. For nonlinear problem there are four additional order conditions that are not encoded in the fourth order stability polynomials [17, Sect. II.1]. This issue is overcome by using a composition of a $s-4$ stage method (based on recurrence relation) with a general

fourth order method having $w_4(z)$ as stability function such that the resulting one-step method has fourth order accuracy for general problems. The Butcher group theory [10] is the fundamental tool to achieve this construction. An interesting feature of the ROCK4 methods is that their stability functions include a strip around the *imaginary* axis near the origin. Such a property (important for hyperbolic-parabolic equations) does not hold for second order stabilized Runge-Kutta methods [3].

Implementation and example

Explicit stabilized RK methods are usually implemented with variable step sizes, variable stage orders, a local estimator of the error and an automatic estimation of the Jacobian of the differential equation to be solved [7; 3; 27; 32]. A code based on stabilized Runge-Kutta methods typically comprises the following steps.

Algorithm.

1. *Selection of the stage number.*

   Given Δt_n, the current step size, compute an approximation of the spectral radius ρ of the Jacobian of (1) and choose the stage number s such $s \simeq \sqrt{\frac{\rho \cdot \Delta t_n}{c_p}}$, where c_p is given by (16).

2. *Integration with current stage number and step size.*

   Perform an integration step from $y_n \to y_{n+1}$.

3. *Error estimate and step size adjustment.*

   Compute the local error err_{n+1}. If $err_n \leq Tol$ accept the step size and update the integration time $t \to t + \Delta t_n$, compute a new step size $\Delta t_{n+1} = \xi(err_n, err_{n+1}, \Delta t_{n-1}, \Delta t_n)$ and go back to 1. If $err_n > Tol$ reject the step size, compute a new step size $\Delta t_{n,new} = \xi(err_n, err_{n+1}, \Delta t_{n-1}, \Delta t_n)$ and go back to 1.

The function ξ is a step size controller "with memory" developed for stiff problems [16] and Tol is a weighted average of `atol` (absolute tolerance) and `rtol` (relative tolerance). If the spectral radius Jacobian is not constant or cannot be easily approximated, it is estimated numerically during the integration process through a power like method that takes advantage of the large number of internal stages used for stabilized Runge-Kutta methods.

Example. We consider a chemical reaction, the Brusselator, introduced by Prigogine, Lefever and Nicolis (see for example [17, I.1] for a description), given by the following reaction diffusion equations involving the concentration of two species $u(x,t), v(x,t)$: $\Omega \times (0,T) \longrightarrow \mathbb{R}$

$$\frac{\partial u}{\partial t} = a + u^2 v - (b+1)u + \alpha \Delta u$$
$$\frac{\partial v}{\partial t} = bu - u^2 v + \alpha \Delta v.$$

A spatial discretization (e.g., by finite differences) of the diffusion operator leads to

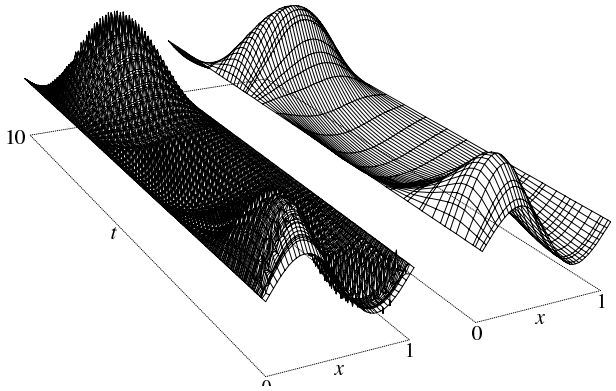

Fig. 6. Integration of the Brusselator problem with the Dorman-Prince method of order 5 (DOPRI5), (left Fig) and the ROCK4 method (right Fig). A few intermediate stages are also displayed for the ROCK4 method.

a large system of ODEs. For illustration purpose, we take $\Omega = (0,1)$ and $t \in (0,10)$. We choose to compare the ROCK4 method with a classical efficient high order explicit

Runge-Kutta method, namely the fifth order method based on Dorman and Prince formulas (DOPRI5). We integrate the problem with the same tolerance for ROCK4 and DOPRI5 and check that we get the same accuracy at the end. The cost of solving the problem is as follows. Number of step sizes: 406 (DOPRI5), 16 (ROCK4), number of function evaluations: 2438 (DOPRI5), 283 (ROCK4).

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