# Two-step modified collocation methods with structured coefficient matrices

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**Abstract**

In the context of the numerical integration of initial value problems based on ordinary differential equations, it is the purpose of this paper to introduce a modification of two step collocation methods, in order to obtain coefficient matrices with a structured shape, to get an efficient implementation. Our aim is the development of new collocation-based methods having high order of convergence and strong stability properties (e.g. $A$-stability and $L$-stability). We present the constructive technique, discuss the order of convergence and the stability properties of the resulting methods and provide some numerical results confirming the theoretical expectations.

*Key words:* Two-step Runge-Kutta methods, almost collocation methods, $A$-stability, $L$-stability, Singly Implicit Runge–Kutta methods, Diagonally Implicit Runge–Kutta methods.

## 1. Introduction

It is the purpose of this paper to approach the numerical solution of Hadamard well-posed systems of ordinary differential equations (ODEs)

$$\begin{cases} y'(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d \end{cases} \tag{1.1}$$

with $f : [t_0, T] \times \mathbb{R}^d \to \mathbb{R}^d$, by means of highly stable multistage integration methods. Because of the implicitness of such methods, the numerical solution of nonlinear systems of equations is strongly involved in the integration process and the computational cost of an implicit numerical method then strictly depends on the computational cost required to solve such nonlinear systems: for this reason, we focus our attention on the development and the analysis of new continuous formulae with structured coefficient matrices. In fact, the solution of linear and nonlinear systems of equations can be efficiently computed if their coefficient matrix shows a structured shape. In this case, some function evaluations can be avoided or the Jacobian of the system can be stored and re-used for a certain number of iterations or a fast computation (e.g. in a parallel environment) can be provided.

In order to derive numerical methods having the mentioned features, we consider a modification of the two-step algebraic collocation technique. Our purpose is to combine the advantages of implicit Runge–Kutta methods depending on a structured coefficient matrix, e.g. efficient solution of the nonlinear system in the stages, with the advantages of multistep collocation methods, i.e. high stage order, uniform order of convergence and strong stability properties.

Two-step collocation methods (1.2) were introduced in [16] and further investigated in [15, 17, 18, 20], also in the context of Volterra integral equations [13, 14]. In this work the solution $y(t_n+sh)$, where $s$ is the time scaled variable, is approximated by means of the algebraic polynomial

$$\begin{cases} P(t_n+sh) = \varphi_0(s)y_{n-1} + \varphi_1(s)y_n \\ \quad + h\displaystyle\sum_{j=1}^{m}\Big(\chi_j(s)f(P(t_{n-1}+c_jh)) + \psi_j(s)f(P(t_n+c_jh))\Big), \\ y_{n+1} = P(t_{n+1}), \end{cases} \tag{1.2}$$

named collocation polynomial, which is formulated as linear combination of the basis polynomials $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$, and $\psi_j(s)$, $j=1,2,\dots,m$. It is usually considered that $s\in[0,1]$, but this restriction is not necessary, at least when we have to evaluate the polynomial $P(t_n+sh)$ in future points: such evaluations occur, for instance, when some of the collocation points $c_i$, $i=1,2,\dots,m$, are greater than 1.

It is generally assumed that the collocation polynomial (1.2) satisfies the interpolation conditions $P(t_{n-1})=y_{n-1}$, $P(t_n)=y_n$ and the collocation conditions $P'(t_{n-1}+c_jh)=f(P(t_{n-1}+c_jh))$, $P'(t_n+c_jh)=f(P(t_n+c_jh))$, $j=1,2,\dots,m$. However, in order to reach strong stability properties (e.g.

$A$-stability, $L$-stability and algebraic stability), we impose only some of these conditions and get rid of all the others, obtaining some degrees of freedom to be spent for the stability purpose. Such methods are denoted as two-step *almost* collocation methods [16].

Setting $Y_j^{[n-1]} = P(t_{n-1} + c_j h)$ and $Y_j^{[n]} = P(t_n + c_j h)$, $j = 1, 2, \ldots, m$, the method (1.2) can be regarded as two-step Runge-Kutta (TSRK) method

$$\begin{cases} y_{n+1} = \theta y_{n-1} + \widetilde{\theta} y_n + h\big((v^T \otimes I_d)F^{[n-1]} + (w^T \otimes I_d)F^{[n]}\big), \\ Y^{[n]} = (u \otimes I_d)y_{n-1} + \big((e-u) \otimes I_d\big)y_n + h\big((A \otimes I_d)F^{[n-1]} + (B \otimes I_d)F^{[n]}\big), \end{cases} \tag{1.3}$$

with

$$\begin{array}{llll} \theta = \varphi_0(1), & \widetilde{\theta} = \varphi_1(1), & v_j = \chi_j(1), & w_j = \psi_j(1), \\ u_i = \varphi_0(c_i), & \widetilde{u}_i = \varphi_1(c_i), & a_{ij} = \chi_j(c_i), & b_{ij} = \psi_j(c_i), \end{array}$$

and where $F^{[n]} = [f_1(Y_1^{[n]}), \ldots, f_1(Y_m^{[n]}), \ldots, f_d(Y_1^{[n]}), \ldots, f_d(Y_m^{[n]})]^T$, $I_d$ is the identity matrix of dimension $d$, $e = [1, \ldots, 1]^T \in \mathbb{R}^m$ and $\otimes$ denotes the usual Kronecker tensor product. In analogous manner, for $s \neq 1$, equation (1.2) can lead to a continuous TSRK method.

The computational cost of a TSRK method (1.3) is strongly related to the solution of the nonlinear system for the computation of $Y^{[n]}$, whose coefficient matrix depends on the matrix $B$. An efficient solution of such system could be provided if $B$ takes a special structure (e.g. triangular or diagonal). Jackiewicz and Tracogna identified in [21] four different types of TSRK methods according to the structure of $B$:

- methods of type 1 and 2, with $B$ lower triangular and having only one nonzero eigenvalue $\lambda$, with $\lambda = 0$ and $\lambda \neq 0$ respectively, suitable to integrate nonstiff and stiff systems respectively in a serial computing environment;

- methods of type 3 and 4, depending on $B = \text{diag}(\lambda, \ldots, \lambda)$, with $\lambda = 0$ and $\lambda \neq 0$ respectively, suitable to integrate nonstiff and stiff systems respectively in a parallel computing environment.

In particular, if $B$ is a full matrix, (1.3) requires the solution of a nonlinear system of dimension $md \times md$; if $B$ is lower triangular, $m$ successive nonlinear systems of dimension $d$ must be solved while, in case of $B$ diagonal, the solution of $m$ independent nonlinear systems of dimension $d$ must be provided. Moreover,

- in the case of type 2 methods, i.e. $B$ lower triangular and one-point spectrum, if the nonlinear system in (1.3) is solved by means of Newton-type iterations, the stored LU-factorization of the coefficient matrix $I_d - h\lambda J_i^{[n]}$ can be repeatedly used for a certain number of iterations, where $J_i^{[n]}$ is the $i$-th block column of the Jacobian of $F^{[n]}$;
- if $B$ is diagonal, a fast resolution of the nonlinear system in a parallel environment can be provided.

The purpose of this paper is the derivation of highly-stable two-step almost collocation methods (1.2) equivalent to TSRK methods (1.3) of type 2 and 4 (see [21]), therefore developing families of diagonally implicit continuous methods, following the lines drawn in the discrete case [1, 3, 4, 5, 6, 8, 9, 10, 11, 19, 20, 22] which led to the classes of DIRK, SDIRK, SIRK and DIMSIMs methods. The paper is structured as follows: Sections 2 and 3 are devoted to analysis of methods with $B$ triangular and diagonal respectively, together with the requirements to fulfill in order to gain the desired structure; Section 4 is focused on the procedure to follow in order to derive highly stable structured formulae (i.e. $A$-stable and $L$-stable) within the class (1.2) and examples of such methods are provided in Section 5; some numerical experiments are performed in Section 6 while in Section 7 some conclusions are given.

## 2. Two-step almost collocation methods with triangular coefficient matrix

We analyze in this section the class of two-step almost collocation methods (1.2) such that the matrix $B$ is lower triangular. Since $B = \big(\psi_j(c_i)\big)_{i,j=1}^{m}$, the conditions to impose in order to enforce a special structure on $B$ strongly involve the basis polynomials $\psi_j(s)$, $j = 1, 2, \ldots, m$. The following result holds.

**Proposition 2.1.** *Assume that the basis functions $\varphi_0(s)$, $\varphi_1(s)$ and $\chi_j(s)$, $j = 1, 2, \ldots, m$, in (1.2) have degree at most $p$ and that the corresponding method is nonconfluent. Then, the matrix $B$ is lower triangular if and only if*

$$\psi_j(s) = \omega_j(s) \prod_{k=1}^{j-1} (s - c_k), \tag{2.1}$$

*where $\omega_j(s)$ is a polynomial of degree less or equal than $p-j+1$, $j = 2, \ldots, m$ and $p$ is the order of the method.*

*Proof*: We suppose $B$ lower triangular: as a consequence, $b_{ij} = 0$ for $i < j$ ($j = 2, \ldots, m$) and, therefore, $\psi_j(c_i) = 0$ for $i < j$ ($j = 2, \ldots, m$). This implies that $c_1, c_2, \ldots, c_{j-1}$ are roots of $\psi_j(s)$, $j = 2, \ldots, m$. Hence, $\psi_j(s)$ can be factorized in the form (2.1), where $\omega_j(s)$ is a polynomial of degree $\deg(\psi_j(s)) - j + 1$, $j = 2, \ldots, m$. However, we infer from the system of order conditions [15, 16]

$$\begin{cases} \varphi_0(s) + \varphi_1(s) = 1, \\ \dfrac{(-1)^k}{k!}\varphi_0(s) + \displaystyle\sum_{j=1}^{m} \left( \chi_j(s) \frac{(c_j - 1)^{k-1}}{(k-1)!} + \psi_j(s) \frac{c_j^{k-1}}{(k-1)!} \right) = \frac{s^k}{k!}, \end{cases} \tag{2.2}$$

with $s \in [0, 1]$ and $k = 1, 2, \ldots, p$, that $\deg(\psi_j(s)) \leq p$, where $p$ is the order of the method. This completes the sufficient part. The necessary part is trivial.

□

We next analyze the order of convergence of the resulting methods. In accordance with proposition 2.1, the system of order conditions (2.2) can be specialized to the case of methods with $B$ lower triangular, as reported in the following result.

**Theorem 2.1.** *A two-step collocation method (1.2) equivalent to a TSRK method (1.3) with $B$ lower triangular has order $p$ if and only if*

$$\begin{cases} \varphi_0(s) + \varphi_1(s) = 1, \\ \dfrac{(-1)^k}{k!}\varphi_0(s) + \displaystyle\sum_{j=1}^{m} \left( \chi_j(s) \frac{(c_j - 1)^{k-1}}{(k-1)!} + \frac{c_j^{k-1}}{(k-1)!} \left( \sum_{\ell=0}^{p-j+1} \alpha_\ell^{(j)} s^\ell \right) \prod_{r=1}^{j-1} (s - c_r) \right) = \frac{s^k}{k!}, \end{cases} \tag{2.3}$$

*with $s \in [0, 1]$, $k = 1, 2, \ldots, p$ and $\alpha_\ell^{(j)} \in \mathbb{R}$, $\ell = 0, \ldots, p-j+1$, $j = 1, \ldots, m$.*

*Proof*: Replace the expression (2.1) for $\psi_j(s)$ in (2.2).

□

The real parameters $\alpha_\ell^{(j)} \in \mathbb{R}$, $\ell = 0, \ldots, p-j+1$, $j = 1, \ldots, m$, can be regarded as free parameters which add degrees of freedom and can be used in order to enforce the corresponding methods to be highly stable (i.e. $A$-stable or $L$-stable), as it will be discussed in Section 4, where the practical construction of highly stable formulae within the discussed classes of methods is pointed out.

As a consequence of the above results, we can state the following corollary regarding the uniform order of convergence of the derived formulae: to be clear, uniform order of convergence $p$ means that the order $p$ is achieved not only in the grid points, but also in any point $t_n + sh$, $s \in [0, 1]$, which is a direct consequence of order conditions (2.3). This property is particularly useful in the variable stepsize implementation of stiff differential systems (see [15, 18]).

**Corollary 2.1.** *A two-step collocation method (1.2) equivalent to a TSRK method (1.3) with B lower triangular has uniform order of convergence at most equal to* $m + 2$.

*Proof*: The order conditions (2.3) form a system of $p + 1$ equations in the $m + 3$ unknowns $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$, $j = 1, 2, \ldots, m$ and $\psi_1(s)$, which is compatible if $p = m + 2$.

□

The result contained in Corollary 2.1 provides an improvement with respect to diagonally-implicit Runge–Kutta methods, whose effective order is $m$, where $m$ is the number of stages: this is due to the fact that Runge–Kutta methods usually do not have high stage order and, therefore, they suffer from the order reduction phenomenon (see [8], page 288) in the integration of stiff systems. Two-step almost collocation methods (such as the ones derived in [15, 16, 17]), instead, have high stage order $q = p$ overall the integration interval and, for this reason, they do not suffer from order reduction in the integration of stiff systems, which is also confirmed by numerical evidences in [15, 17] and, regarding the methods derived in this paper, in Section 6.

Moreover, it is worthy to observe that two-step collocation methods, rather than one-step collocation methods, depend on much more free parameters which can be used in order to create a better balance between high effective order and strong stability properties (e.g. $A$-stability, $L$-stability and also algebraic stability). This is also clear by the examples of methods provided in Section 5.

## 3. Two-step almost collocation methods with diagonal coefficient matrix

We now consider the properties of two-step almost collocation methods (1.2) equivalent to TSRK methods (1.3) with $B$ diagonal, presenting the main results following the lines drawn in Section 2. We first provide the analytical expression of the polynomials $\psi_j(s)$, $j = 1, 2, \ldots, m$, which enforces the diagonal structure of $B$.

**Proposition 3.1.** *Assume that the basis functions $\varphi_0(s)$, $\varphi_1(s)$ and $\chi_j(s)$, $j = 1, 2, \ldots, m$, in (1.2) have degree at most $p$ and that the corresponding method is nonconfluent. Then, the matrix $B$ is diagonal if and only if*

$$\psi_j(s) = \omega_j(s) \prod_{\substack{k=1 \\ k\neq j}}^{m} (s - c_k), \tag{3.1}$$

*where $\omega_j(s)$ is a polynomial of degree less or equal than $p - m + 1$, $j = 1, 2, \ldots, m$ and $p$ is the order of the method.*

When the matrix $B$ is diagonal, i.e. when the functions $\psi_j(s)$ assume the expression (3.1), the set of order conditions (2.2) takes the following form.

**Theorem 3.1.** *A two-step collocation method (1.2) equivalent to a TSRK method (1.3) with $B$ diagonal has order $p$ if and only if*

$$\begin{cases} \varphi_0(s) + \varphi_1(s) = 1, \\ \dfrac{(-1)^k}{k!}\varphi_0(s) + \displaystyle\sum_{j=1}^{m} \left( \chi_j(s) \frac{(c_j - 1)^{k-1}}{(k-1)!} + \frac{c_j^{k-1}}{(k-1)!} \left( \sum_{\ell=0}^{p-m+1} \mu_\ell^{(j)} s^\ell \right) \prod_{\substack{r=1 \\ r\neq j}}^{m} (s - c_r) \right) = \dfrac{s^k}{k!}, \end{cases} \tag{3.2}$$

*with $s \in [0, 1]$, $k = 1, 2, \ldots, p$ and $\mu_\ell^{(j)} \in \mathbb{R}$, $\ell = 0, \ldots, p-m+1$, $j = 1, \ldots, m$.*

Also in this case, the real parameters $\mu_\ell^{(j)} \in \mathbb{R}$, $\ell = 0, \ldots, p - m + 1$, $j = 1, \ldots, m$, can be regarded as degrees of freedom to use in order to obtain highly stable methods: this is the object of investigation in Section 4. We conclude with the following result concerning the order of convergence of the considered methods, which is a direct consequence of Theorem 3.1.

**Corollary 3.1.** *A two-step collocation method (1.2) equivalent to a TSRK method (1.3) with $B$ diagonal has uniform order of convergence at most equal to $m + 1$.*

## 4. Construction of highly stable formulae

We now focus our attention on the procedures to follow in order to construct highly stable two-step almost collocation methods (1.2) of order $p$ corresponding to TSRK methods (1.3) with $B$ lower triangular or diagonal, according to the considerations reported in Section 2 and 3. The derivation of highly stable methods is a nontrivial task, especially if we ask to create a reasonable balance between high effective order and strong stability properties. For this reason, in order to obtain highly-stable methods, we neglect some order conditions, obtaining some free parameters to be used to gain $A$-stability and $L$-stability. The number $r$ of refused order conditions is what we call *relaxation index*. In the remainder of this section, we address the aspects regarding the construction of $A$-stable and $L$-stable methods of order $p = m + 2 - r$, with $r = 0, 1, 2$ (i.e. methods of order $m + 2$, $m + 1$ or $m$), within the class (1.2) corresponding to TSRK methods (1.3) with $B$ lower triangular, and of order $p = m + 1 - r$, with $r = 0, 1$ (i.e. methods of order $m + 1$ or $m$) and $B$ diagonal.

### *4.1. Construction of methods with B lower triangular*

First of all, we distinguish the following cases:

- if $r = 0$, we assume $\psi_j(s)$, $j = 2, \ldots, m$, of the form (2.1) with

$$\omega_j(s) = \alpha_0^{(j)} + \alpha_1^{(j)} s + \ldots + \alpha_{p-j+1}^{(j)} s^{p-j+1}; \tag{4.1}$$

- if $r = 1$, we consider $\omega_j(s)$, $j = 2, \ldots, m$, of the form (4.1) and set

$$\varphi_0(s) = \beta_0 + \beta_1 s + \ldots + \beta_p s^p; \tag{4.2}$$

- if $r = 2$, we consider $\omega_j(s)$ and $\varphi_0(s)$ of the form (4.1) and (4.2) and set

$$\psi_1(s) = \gamma_0 + \gamma_1 s + \ldots + \gamma_p s^p. \tag{4.3}$$

As we have observed in Section 1, it is generally assumed that the collocation polynomial satisfies some interpolation and/or collocation conditions, selected from the following (compare [15, 16]):

$$\begin{aligned} P(t_{n-1}) &= y_{n-1}, \quad & P'(t_{n-1} + c_j h) &= f(P(t_{n-1} + c_j h)), \\ P(t_n) &= y_n, & P'(t_n + c_j h) &= f(P(t_n + c_j h)), \end{aligned} \tag{4.4}$$

for $j = 1, 2, \ldots, m$. Therefore, we choose from (4.4) some interpolation and/or collocation conditions to impose. These conditions can be expressed in terms of the basis functions $\varphi_0(s)$, $\varphi_1(s)$, $\chi_j(s)$, $\psi_j(s)$, $j = 1, 2, \ldots, m$ as follows:

$$\varphi_0(-1) = 1, \varphi_0'(c_i - 1) = 0, \varphi_0(0) = 0, \varphi_0'(c_i) = 0, \tag{4.5}$$

$$\varphi_1(-1) = 0, \varphi_1'(c_i - 1) = 0, \varphi_1(0) = 1, \varphi_1'(c_i) = 0, \tag{4.6}$$

$$\chi_j(-1) = 0, \chi_j'(c_i - 1) = \delta_{ij}, \chi_j(0) = 0, \chi_j'(c_i) = 0, \tag{4.7}$$

$$\psi_j(-1) = 0, \psi_j'(c_i - 1) = 0, \psi_j(0) = 0, \psi_j'(c_i) = \delta_{ij}, \tag{4.8}$$

where $\delta_{ij}$ is the usual Kronecker delta, $i, j = 1, 2, \ldots, m$.

We next derive the values of some $\alpha_\ell^{(j)}$, $\beta_i$, $\gamma_i$, for $\ell = 0, 1, \ldots, p - j + 1$ and $i = 0, 1, \ldots, p$, in such a way that the chosen conditions are satisfied on the fixed functions $\omega_j(s), \varphi_0(s)$ and/or $\varphi_1(s)$, according to the value of the relaxation index $r$. We next solve the system of order conditions (2.2) up to $p$, with respect to the remaining basis functions: they automatically inherit the same interpolation/collocation conditions imposed, as proved in [16, 20] for any two-step collocation method within the class (1.2).

If in addition to the triangular structure for $B$ we also require it to be one point spectrum, i.e. we ask for two-step almost collocation formulae (1.2) equivalent to type 2 TSRK methods (1.3), we spend some of the remaining free parameters within the set of $\alpha_\ell^{(j)}$ and $\gamma_i$, for $\ell = 0, 1, \ldots, p - j + 1$ and $i = 0, \ldots, p$, in order to equal all the values on the diagonal of $B$, i.e. all the $\psi_j(c_j)$, $j = 1, \ldots, m$, equal to a correspond to a real common value $\lambda$.

We next compute the stability matrix $M(z)$ (compare [15, 16, 20]) and derive the corresponding stability polynomial, i.e. the characteristic polynomial of $M(z)$

$$p(\eta, z) = \det\left(I_{m+2} - \eta M(z)\right) = \sum_{k=0}^{m+2} p_k(z)\eta^k, \tag{4.9}$$

of degree $m + 2$ with respect to $\eta$, where $p_k(z)$ is a rational function in $z$, $k = 0, 1, \ldots, m+2$. If possible, we spend some of the free parameters in order to reduce the degree of $p(\eta, z)$ with respect to $\eta$ (e.g. to obtain a quadratic stability polynomial, compare [12]). Let us suppose that the resulting degree of $p(\eta, z)$ with respect to $\eta$ is $\nu$.

Using the Schur criterion (compare [23]), we determine the values of the remaining parameters corresponding to $A$-stable methods. If the corresponding set of $A$-stable methods is nonempty, we search for the related subset of $L$-stable methods, solving the nonlinear system

$$\begin{cases} \lim\limits_{z\to-\infty} \dfrac{p_0(z)}{p_\nu(z)} = 0, \\ \vdots \\ \lim\limits_{z\to-\infty} \dfrac{p_{\nu-1}(z)}{p_\nu(z)} = 0. \end{cases} \tag{4.10}$$

*4.2. Construction of methods with B diagonal*

In order to obtain a diagonal shape for the matrix $B$, together with strong stability properties, we proceed as follows. We distinguish the following cases:

- if $r = 0$, we assume $\psi_j(s)$, $j = 1, \ldots, m$, of the form (3.1) with

$$\omega_j(s) = \mu_0^{(j)} + \mu_1^{(j)} s + \ldots + \mu_{p-m+1}^{(j)} s^{p-m+1}; \tag{4.11}$$

- if $r = 1$, we consider $\omega_j(s)$, $j = 1, \ldots, m$, of the form (4.11) and set

$$\varphi_0(s) = \sigma_0 + \sigma_1 s + \ldots + \sigma_p s^p. \tag{4.12}$$

We next impose some interpolation and/or collocation conditions on the functions fixed above, chosen from the sets (4.5) and (4.8), i.e. we derive the values of some $\mu_\ell^{(j)}$, $\sigma_i$, for $\ell = 0, 1, \ldots, p-m+1$ and $i = 0, 1, \ldots, p$, in such a way that these conditions are satisfied. Then, we solve the system of order conditions (2.2) up to $p$, with respect to the remaining basis functions: they automatically inherit the interpolation/collocation conditions imposed, as proved in [16, 20] for any two-step collocation method within the class (1.2).

If in addition to the diagonal structure for $B$ we also require it to be one point spectrum, i.e. we ask for two-step almost collocation formulae (1.2) equivalent to type 4 TSRK methods (1.3), we spend some of the remaining free parameters within the set of $\mu_\ell^{(j)}$, for $\ell = 0, 1, \ldots, p-m+1$, in order to equal all the values on the diagonal of $B$, i.e. all the $\psi_j(c_j)$, $j = 1, \ldots, m$, equal to a correspond to a real common value $\lambda$.

We next compute the stability polynomial (4.9) of degree $m+2$ with respect to $\eta$, where $p_k(z)$ is a rational function in $z$, $k = 0, 1, \ldots, m+2$. If possible, we spend some of the free parameters in order to reduce the degree of $p(\eta, z)$ with respect to $\eta$ (e.g. to obtain a quadratic stability polynomial, compare [12]). Let us suppose that the resulting degree of $p(\eta, z)$ with respect to $\eta$ is $\rho$. Using the Schur criterion, we determine the values of the remaining parameters corresponding to $A$-stable methods. If the corresponding set of $A$-stable methods is nonempty, we search for the related subset of $L$-stable methods, solving the nonlinear system

$$\begin{cases} \displaystyle\lim_{z \to -\infty} \frac{p_0(z)}{p_\rho(z)} = 0, \\ \qquad \vdots \\ \displaystyle\lim_{z \to -\infty} \frac{p_{\rho-1}(z)}{p_\rho(z)} = 0. \end{cases} \tag{4.13}$$

## 5. Examples of methods

We now provide some examples of two-step almost collocation methods (1.2) with $m = 2$, equivalent to TSRK methods (1.3) with structured $B$, according to the issues provided in Section 4 and, in particular, taking into account what follows. In principle, we could impose all the conditions (4.5-4.8) but, as also observed in previous papers (see [15,16]), poor stability properties are reached. Therefore, we decide to impose just some of the conditions among (4.5-4.8), assuming to interpolate in 0, more than in $-1$, and collocate in some $c_i$, more than in $c_i - 1$ because, in the practice, these choices generally lead to $A$-stability, more than the conditions involving points located in the past (e.g. $-1$ and $c_i - 1$). These lines will now be drawn in the effective construction of the methods, as follows.

### *5.1. Analysis of methods with $m = 2$ and $B$ lower triangular*

Applying the Schur criterion, it is possible to prove that no $A$-stable methods with $m = 2$ and maximum attainable uniform order $p = 4$ exist and, therefore, we relax one order condition, in order to find highly stable methods within the class (1.2) with $m = 2$ and $p = m + 1 = 3$, corresponding to TSRK methods (1.3) with $B$ lower triangular. Since $r = 1$, we assume $\omega_2(s)$ of the form

$$\omega_2(s) = \alpha_0 + \alpha_1 s + \alpha_2 s^2, \tag{5.1}$$

and $\varphi_0(s)$ of the type

$$\varphi_0(s) = \beta_0 + \beta_1 s + \beta_2 s^2 + \beta_3 s^3. \tag{5.2}$$

We next impose some the interpolation and collocation conditions among (4.5-4.8). In particular, we choose

$$\varphi_0(0) = 0,\ \varphi_0'(c_2) = 0,\ \psi_2(0) = 0,\ \psi_2'(c_2) = 1,$$

obtaining

$$\alpha_0 = 0, \quad \alpha_2 = \frac{1 + c_1\alpha_1 - 2c_2\alpha_1}{c_2(-2c_1 + 3c_2)}, \quad \beta_0 = 0, \quad \beta_3 = -\frac{\beta_1 + 2c_2\beta_2}{3c_2^2}.$$

As a consequence, a five-parameter family of methods (1.2) arises: the degrees of freedom are $c_1, c_2, \alpha_1, \beta_1, \beta_2$. We next compute the stability polynomial (4.9), which assumes the form

$$p(\eta, z) = \eta(p_0(z) + p_1(z)\eta + p_2(z)\eta^2 + p_3(z)\eta^3),$$

and compute the values of $\beta_2$ and $c_2$ annihilating $p_0(z)$, in such a way that the stability properties of the related methods depend on the quadratic stability function

$$\widetilde{p}(\eta, z) = p_1(z) + p_2(z)\eta + p_3(z)\eta^2. \tag{5.3}$$

These values are

$$\beta_2 = \frac{-\beta_1(c_1 + 6\alpha_1 - 6c_1\alpha_1 - 2c_1^2\alpha_1 + 2c_1^3\alpha_1)}{2c_1\alpha_1(3 - 5c_1 + 2c_1^2)}, \quad c_2 = 1.$$

We next apply the Schur criterion on the polynomial (5.3) in correspondence of

$$\beta_1 = \frac{6c_1\alpha_1(-1 + c_1)}{2 + 3c_1}$$

achieving $L$-stability, i.e. solving the system (5.4) which, for the polynomial (5.3), takes the form

$$\begin{cases} \lim\limits_{z\to-\infty} \dfrac{p_1(z)}{p_3(z)} = 0, \\ \lim\limits_{z\to-\infty} \dfrac{p_1(z)}{p_3(z)} = 0. \end{cases} \tag{5.4}$$

Applying the Schur criterion we are able to find the values of the remaining free parameters $c_1$ and $\alpha_1$ corresponding to $A$-stable and, in particular, $L$-stable methods. The results are given in Figure 1. The region provided in

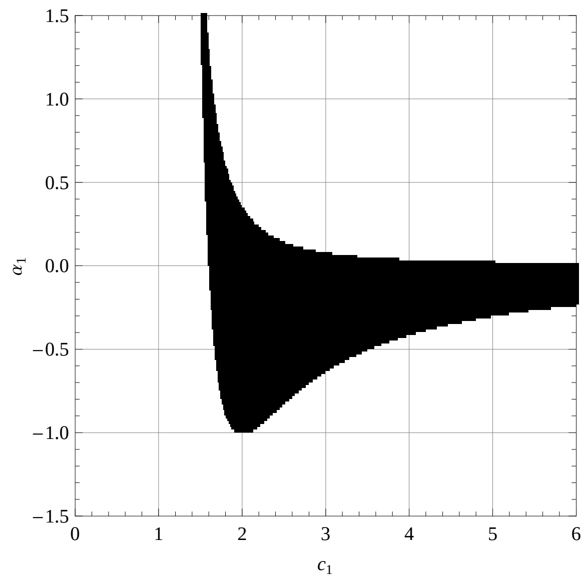


Figure 1: Region of $L$-stability in the $(c_1, \alpha_1)$-plane for diagonally implicit two-step almost collocation methods (1.2), with $m = 2$ and $p = 3$

Figure 1 arises from the union of the following sets:

$$\Sigma_1 = \left\{(c_1,\alpha_1)\in\mathbb{R}^2 : \frac{1+\sqrt{17}}{4} < c_1 < \frac{3}{2},\ \frac{1}{5-9c_1+4c_1^2} < \alpha_1 < \frac{1+c_1-c_1^2}{(-1+c_1)^3}\right\},$$

$$\Sigma_2 = \left\{(c_1,\alpha_1)\in\mathbb{R}^2 : \frac{3}{2} < c_1 \leq \frac{1+\sqrt{5}}{2},\ \frac{1+c_1-c_1^2}{(c_1-1)^3} < \alpha_1 < \frac{1}{4c_1^2-9c_1+5}\right\},$$

$$\Sigma_3 = \left\{(c_1,\alpha_1)\in\mathbb{R}^2 : c_1 > \frac{1+\sqrt{5}}{2},\ \frac{-c_1^2+c_1+1}{(c_1-1)^3} < \alpha_1 < 0\right\},$$

$$\Sigma_4 = \left\{(c_1,\alpha_1)\in\mathbb{R}^2 : c_1 > \frac{1+\sqrt{5}}{2},\ 0 < \alpha_1 < \frac{1}{4c_1^2-9c_1+5}\right\}.$$

We observe from Figure 1 that, at least in the methods we have derived, $A$-stability is reached only in correspondence of collocation points greater than 1 and, therefore, extrapolation is involved. Anyway, as it can also be experimentally observed in Section 6, this does not deteriorate the accuracy of the resulting methods.

If we aim for two-step almost collocation methods (1.2) equivalent to type 2 TSRK methods (1.3), we apply the same procedure above described but, instead of spending some parameters to reduce the degree of the stability polynomial, we use them to obtain equal values on the diagonal of the matrix $B$. For this reason, after computing $\alpha_0,\ \alpha_2,\ \beta_0,\ \beta_3$ as above, we determine the value of $\beta_2$ such that $b_{11} = b_{22}$, obtaining

$$\beta_2 = \frac{-3(2c_1^3 - 6(1+\alpha_1) - 3c_1^2(3+2\alpha_1) + 3c_1(5+4\alpha_1))}{c_1(-1+3c_1)(3-2c_1)^2},$$

in correspondence of the values $c_2 = \frac{3}{2}$ and $\beta_1 = 0$. This values are chosen in order to simplify the structure of the stability polynomial, whose stability properties are analyzed using the Schur criterion. The results of this analysis are reported in Figure 2.

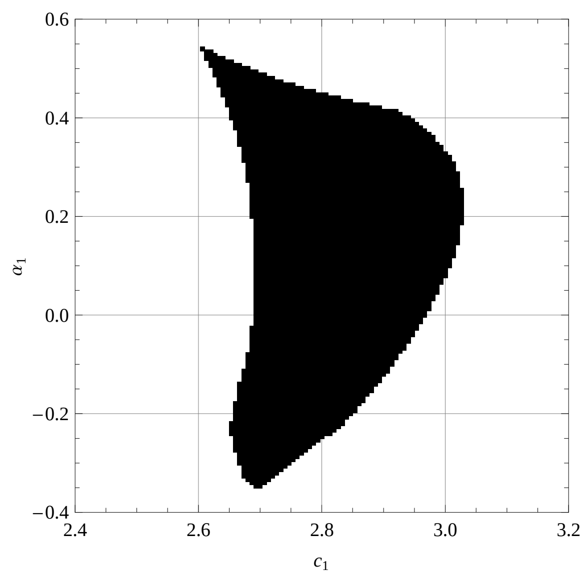


Figure 2: Region of $A$-stability in the $(c_1, \alpha_1)$-plane for type 2 two-step almost collocation methods (1.2), with $m = 2$ and $p = 3$, for $c_2 = \frac{3}{2}$ and $\beta_1 = 0$

*5.2. Analysis of methods with $m = 2$ and $B$ diagonal*

We conclude this section deriving highly stable two-step almost collocation methods (1.2) with $m = 2$, equivalent to type 4 TSRK methods (1.3).

It possible to prove, applying the Schur criterion, that no $A$-stable type 4 almost collocation methods (1.2) of order $m = 2$ and $p = 3$ exist and, therefore, we relax one order condition, searching for methods of order $p = m = 2$. We assume that

$$\omega_1(s) = \mu_0^{(1)} + \mu_1^{(1)} s, \quad \omega_2(s) = \mu_0^{(2)} + \mu_1^{(2)} s, \quad \varphi_0(s) = \sigma_0 + \sigma_1 s + \sigma_2 s^2,$$

and, among (4.5-4.8), we have chosen the interpolation conditions

$$\varphi_0(0) = 0, \quad \psi_1(0) = 0, \quad \psi_2(0) = 0,$$

obtaining $\mu_0^{(1)} = \mu_0^{(2)} = \sigma_0$. Six free parameters are left, i.e. $\mu_1^{(1)}, \mu_2^{(1)}, \sigma_1, \sigma_2, c_1$ and $c_2$. We set $\mu_1^{(1)} = \mu_2^{(1)} = 1$ and derive the values of $\sigma_1, \sigma_2$ and $c_2$ solving the system (4.13) for $L$-stability, obtaining

$$\sigma_1 = -\frac{2(7c_1^3 - 8c_1^2 - 9c_1 + 2)}{4c_1^2 - 3c_1 + 3}, \quad \sigma_2 = \frac{4c_1^3 + 4c_1^2 - 23c_1 + 3}{4c_1^2 - 3c_1 + 3}, \quad c_2 = 1.$$

Applying the Schur criterion we obtain that the resulting methods are $L$-stable if and only if $c_1 \in (-\frac{2}{5}, \frac{270}{619})$.

## 6. Numerical results

In this section we present some numerical evidences arising from the application of the methods derived in Section 5, in order to confirm the theoretical expectations. In particular, we aim to provide an experimental confirmation that, since the derived methods have high stage order (equal to the order of convergence), they do not suffer from order reduction in the integration of stiff differential systems, which is the case for classical Runge-Kutta formulae. In fact, the stage order of Runge–Kutta methods is only equal to $m$, where $m$ is the number of stages. To illustrate these features we compare the following numerical methods:

- TS3: $A$-stable two-step almost collocation method (1.2), with $m = 2$ and

$$\begin{aligned} \varphi_0(s) &= s^2\left(\tfrac{10s}{93} - \tfrac{15}{62}\right), & \varphi_1(s) &= -\tfrac{10s^3}{93} + \tfrac{15s^2}{62} + 1, \\ \chi_1(s) &= -s\left(\tfrac{29s^2}{837} + \tfrac{131s}{620} - \tfrac{2}{5}\right), & \chi_2(s) &= s\left(\tfrac{1804s^2}{4185} - \tfrac{1196s}{775} + \tfrac{43}{25}\right), \\ \psi_1(s) &= s\left(\tfrac{7s^2}{45} - \tfrac{133s}{300} + \tfrac{7}{25}\right), & \psi_2(s) &= -s\left(\tfrac{4s^2}{9} + \tfrac{23s}{15} - \tfrac{3}{5}\right), \end{aligned}$$

of order 3 and stage order 3, equivalent to the type 2 TSRK method

$$
\begin{array}{c|cc|cc}
\frac{45}{62} & -\frac{29}{124} & \frac{451}{155} & \frac{21}{20} & 0 \\
-\frac{45}{248} & -\frac{599}{2480} & \frac{436}{775} & -\frac{21}{400} & \frac{21}{20} \\
\hline
-\frac{25}{186} & -\frac{3739}{16740} & \frac{12719}{20925} & -\frac{7}{900} & \frac{22}{45}
\end{array}, \qquad c = [3, \tfrac{3}{2}]^T;
$$

the method has been obtained in correspondence of the point $(c_1, \alpha_1) = (3, \frac{2}{10})$ of the shaded region reported in Figure 2.

- SDIRK3: two-stage singly diagonally implicit Runge–Kutta method [7]

$$
\begin{array}{c|cc}
(3+\sqrt{3})/6 & (3+\sqrt{3})/6 & 0 \\
(3-\sqrt{3})/6 & -\sqrt{3}/3 & (3+\sqrt{3})/6 \\
\hline
 & 1/2 & 1/2
\end{array}
$$

of order 3 and stage order 2.

We apply these methods to the the van der Pol oscillator (see VDPOL problem in [19])

$$
\begin{cases} y_1' = y_2, & y_1(0) = 2, \\ y_2' = \big((1-y_1^2)y_2 - y_1\big)/\epsilon, & y_2(0) = -2/3, \end{cases} \tag{6.1}
$$

$t \in [0, 3/4]$, with stiffness parameter $\epsilon$. This problem is observed in the interval $[0, 3/4]$, i.e. for the slowly varying parts of the solution, where the problem is stiff for small values of the parameter $\epsilon$ (the problem is not stiff on the interval where the solution is changing rapidly).

We have implemented both methods with a fixed stepsize $h = (T - t_0)/2^k$, for several integer values of $k$, and listed norms of errors $\|e_h^{\text{TS3}}(T)\|$ and $\|e_h^{\text{SDIRK3}}(T)\|$ at the endpoint of integration $T$ and the observed order of convergence $p$. We also report the number $fe$ of function evaluations required by both methods, for each value of the stepsize of integration.

We can observe that for the values of $\epsilon = 10^{-1}$ and $\epsilon = 10^{-3}$ for which the problem (6.1) is not stiff and mildly stiff both methods are convergent with expected order $p = 3$. However, for small values of $\epsilon$ ($\epsilon = 10^{-6}$) for which the van der Pol oscillator is stiff the SDIRK3 method exhibits order reduction phenomenon and its order of convergence drops to about $p = 2$

| $k$ | $\epsilon = 10^{-1}$ | | | $\epsilon = 10^{-3}$ | | | $\epsilon = 10^{-6}$ | | |
|---|---|---|---|---|---|---|---|---|---|
| | $\|e_h^{\mathrm{SDIRK3}}\|$ | $p$ | $fe$ | $\|e_h^{\mathrm{SDIRK3}}\|$ | $p$ | $fe$ | $\|e_h^{\mathrm{SDIRK3}}\|$ | $p$ | $fe$ |
| 8 | $3.41 \cdot 10^{-8}$ | | 2044 | $1.06 \cdot 10^{-4}$ | | 2048 | $2.29 \cdot 10^{-4}$ | | 2174 |
| 9 | $4.49 \cdot 10^{-9}$ | 2.92 | 4066 | $2.00 \cdot 10^{-5}$ | 2.40 | 4096 | $5.85 \cdot 10^{-5}$ | 1.97 | 4156 |
| 10 | $5.78 \cdot 10^{-10}$ | 2.95 | 6406 | $3.31 \cdot 10^{-6}$ | 2.59 | 8192 | $1.47 \cdot 10^{-5}$ | 1.98 | 8192 |
| 11 | $7.52 \cdot 10^{-11}$ | 2.94 | 12288 | $4.92 \cdot 10^{-7}$ | 2.74 | 16382 | $3.69 \cdot 10^{-6}$ | 1.99 | 16384 |
| 12 | $9.81 \cdot 10^{-12}$ | 2.93 | 24576 | $6.80 \cdot 10^{-8}$ | 2.85 | 27610 | $9.27 \cdot 10^{-7}$ | 2.00 | 32768 |

Table 6.1: Numerical results for SDIRK3 method on the Van der Pol oscillator

| $k$ | $\epsilon = 10^{-1}$ | | | $\epsilon = 10^{-3}$ | | | $\epsilon = 10^{-6}$ | | |
|---|---|---|---|---|---|---|---|---|---|
| | $\|e_h^{\mathrm{TS3}}\|$ | $p$ | $fe$ | $\|e_h^{\mathrm{TS3}}\|$ | $p$ | $fe$ | $\|e_h^{\mathrm{TS3}}\|$ | $p$ | $fe$ |
| 8 | $2.38 \cdot 10^{-7}$ | | 2040 | $1.13 \cdot 10^{-6}$ | | 2122 | $1.33 \cdot 10^{-6}$ | | 2550 |
| 9 | $3.02 \cdot 10^{-8}$ | 2.97 | 4084 | $1.65 \cdot 10^{-7}$ | 2.78 | 4090 | $1.87 \cdot 10^{-7}$ | 2.83 | 4486 |
| 10 | $3.82 \cdot 10^{-9}$ | 2.98 | 8110 | $2.29 \cdot 10^{-8}$ | 2.85 | 8184 | $2.47 \cdot 10^{-8}$ | 2.92 | 8428 |
| 11 | $4.81 \cdot 10^{-10}$ | 2.99 | 13724 | $3.05 \cdot 10^{-9}$ | 2.91 | 16376 | $3.17 \cdot 10^{-9}$ | 2.96 | 16404 |
| 12 | $6.01 \cdot 10^{-11}$ | 3.00 | 24570 | $3.74 \cdot 10^{-10}$ | 3.03 | 32760 | $3.78 \cdot 10^{-10}$ | 3.07 | 32760 |

Table 6.2: Numerical results for TS3 on the Van der Pol problem

which corresponds to the stage order $q = 2$. This is not the case for TS3 method which preserves order of convergence $p = q = 3$, which leads to higher accuracy.

Moreover, we also observe that, in each considered case, the computational cost of both TS3 and SDIRK3 methods is essentially the same. Therefore, on the analyzed problem, the method TS3 behaves as SDIRK3 in terms of computational cost, but achieves an higher accuracy.

## 7. Concluding remarks

In this paper we have derived and analyzed a family of $A$-stable and $L$-stable methods belonging to the class of two-step collocation methods (1.2), equivalent to TSRK methods (1.3), with structured coefficient matrices. The derived methods combine the advantages of implicit Runge–Kutta methods depending on a structured coefficient matrix with the ones of multistep collocation methods, e.g. high effective order of convergence, strong stability (e.g. $A$-stability and $L$-stability), possibility to assess an easy strategy to change the stepsize of integration (see [15, 18]).

Even if $A$-stable discrete TSRK methods (1.3) depending on a structured coefficient matrix $B$ already exist in the literature (see, for instance, the paper [21]), it is worthy to observe that those methods are not based on collocation and, therefore, they do not benefit of the advantages of continuous methods, e.g. an uniform order of convergence (with consequent high effective order) and the possibility of easily changing the stepsize in a variable stepsize implementation: in fact, we can easily recognize the missing approximations which are needed when advancing along the grid by evaluating the piecewise approximant (1.2) in the needed points, as already done in [15, 18]).

These methods are useful for an efficient implementation, as our first numerical experiments show and as it happened for the analogous one-step methods. In future works, we intend to exploit the mentioned features, in order to carry out a variable stepsize-variable order implementation, also in parallel environment, of the derived two-step collocation methods.

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