Partitioned Runge-Kutta Methods for Semi-explicit Differential-Algebraic Systems of Index 2

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Abstract

A general class of one-step methods for index 2 differential-algebraic systems in Hessenberg form is studied. This family of methods, which we call partitioned Runge-Kutta methods, includes all one-step methods of Runge-Kutta type proposed in the literature for integrating such DAE systems, including the more recently proposed classes of half-explicit methods. A new family of super-convergent partitioned Runge-Kutta methods based on Gauss methods is presented. A detailed theoretical study of partitioned Runge-Kutta methods that exactly satisfy the original algebraic constraint of the DAE system is given. In particular, methods with different order of convergence for the differential variables and the algebraic variables are also studied using a graph theoretical approach.

Keywords: Differential-algebraic systems of index 2, half-explicit Runge-Kutta methods, partitioned Runge-Kutta methods, order conditions, trees.

1 Introduction

We consider semi-explicit systems of differential-algebraic equations of index 2 given in autonomous and Hessenberg form

$$y' = f(y, z), \quad 0 = g(y), \tag{1}$$

where f and g are assumed to be sufficiently differentiable and

$$g_y(y)f_z(y,z) \text{ is invertible} \tag{2}$$

in a neighborhood of the solution. The initial values (y_0, z_0) are required to be consistent, i.e., satisfy the consistency equations

$$g(y_0) = 0, \tag{3}$$
$$g_y(y_0)f(y_0, z_0) = 0. \tag{4}$$

Problems of the form (1) are frequently encountered in practice (multi-body systems, nonlinear control, etc). In the last years, much attention has been paid to the development and analysis of numerical methods for the integration of such systems (see [5, 11]).

The system (1) can be integrated considering the system obtained from (1) differentiating once the constraint, i.e., the index 1 DAE

$$y' = f(y,z), \quad 0 = g_y(y)f(y,z). \tag{5}$$

In that case, the application of some stabilization technic is recommended. Here, we are concerned with one-step methods that directly integrate the problem (1), without making use of the algebraic constraints of (5) (the so called hidden constraints). The first one-step methods for integrating directly the system (1) studied in the literature are implicit Runge-Kutta methods [6, 9] (see also [5, 11]). Half-explicit Runge-Kutta methods, proposed in [9] and developed in [3, 2, 4] allows to solve more efficiently certain problems of the form (1) arising in the simulation of multi-body systems in (index 2) descriptor form. Arnold [1] and the present author [13] have independently considered new classes of half-explicit methods to integrate directly (1) that seem to be more efficient than the older ones; moreover, unlike those first half-explicit methods, accurate approximations of the algebraic variable z are also provided by the new methods. A new family of one-step implicit methods for solving (1) methods is presented in Subsection 6.2. These methods, which we call *Gauss-Lobatto* methods, based on Gauss methods, are symmetric and a s-stage method provide, for the differential variable y, $2s$th order approximations that satisfy the algebraic constraint of (1).

All the abovementioned methods belong to the general family of partitioned Runge-Kutta methods we present in Section 2. For most one-step methods for integrating directly the problem (1) considered in the literature, only the approximation y_n of the differential variable y is needed to advance each integration step of the method. We say that a one-step method to solve (1) is, of *type 1* if y_{n+1} does not depend on z_n, and of *type 2* otherwise. The implicit Runge-Kutta methods based on Gauss and Radau quadrature formulas, as well as the half-explicit Runge-Kutta methods proposed in [9] are of type 1. The Gauss-Lobatto methods we present in Subsection 6.2 are also of this first type. Well known examples of type 2 methods are the implicit Runge-Kutta LobattoIIIA methods (whose convergence properties for the application to the system (1) were studied in detail by [12]). The new half-explicit methods proposed in [1] and [13] also belong to this second type.

The existence and influence of perturbations of partitioned Runge-Kutta methods is studied in detail in Section 3. Section 4 is devoted to the convergence study of partitioned Runge-Kutta methods that provides approximations that exactly satisfy the algebraic constraints of (1). Here, characterizations of the convergence of the methods in terms of the Taylor expansions of the local errors, and in the case of methods of type 2, the expansion of $\partial y_{n+1}/\partial z_n$ are obtained. In Section 5, algebraic characterizations (in terms of the parameters of the method) of the convergence conditions obtained in previous section are obtained. The Taylor expansions of the local errors and $\partial y_{n+1}/\partial z_n$ are obtained in a systematic way using trees (the same trees used in [9, 11] in the case of the local errors).

Section 6 is devoted to the construction of PRK methods which satisfy exactly the constraints of (1). Here, a fundamental role will be played by certain generalizations of the usual simplifying assumptions devised by Butcher [7] (see also [10]) for Runge-Kutta methods for ODEs, and extended for index 2 DAEs in [9]. Some basic simplifying assumptions, which will be used in the rest of the present section, are presented in the first subsection. Subsection 6.2 is devoted to a subclass of PRK methods obtained as an extension of collocation methods for index 2 DAEs (see Definition VI.7.7 of [11]). In particular, the new family of *Gauss-Lobatto* methods, a class of symmetric s-stage implicit methods of order $2s$ (for the differential variables), are presented. Results based on simplifying assumptions to construct high order implicit PRK methods of type 1 and type 2 are respectively obtained in Subsection 6.3 and 6.4. In Subsection 6.5, the *partitioned half-explicit Runge-Kutta* methods proposed in [13] are studied.

2 Partitioned Runge-Kutta methods

In [13] we propose a general class of methods to solve the system of DAEs (1), the *partitioned Runge-Kutta methods* (PRK):

$$\begin{aligned} i &= 1,\ldots,s, \\ & \qquad Y_i = y_0 + h\sum_{j=1}^{s} a_{ij} f(Y_j,Z_j), \\ & \qquad \overline{Y}_i = y_0 + h\sum_{j=1}^{s} \bar{a}_{ij} f(Y_j,Z_j), \quad g(\overline{Y}_i) = 0 \qquad (6) \\ y_1 &= \sum_{i=1}^{s} b_i f(Y_i,Z_i), \quad z_1 = \sum_{i=1}^{s} d_i Z_i. \end{aligned}$$

We denote as A and $\bar{A}$ the $s \times s$ matrices with entries a_{ij} and $\bar{a}_{ij}$ respectively, and $b = (b_1, \dots, b_s)^T$, $d = (d_1, \dots, d_s)^T$

Of particular interest are PRK methods (6) such that

$$b_i = \bar{a}_{ki} \ (1 \leq i \leq s) \text{ for some } k, \tag{7}$$

so that $y_1 = \bar{Y}_k$, and therefore the numerical solution y_1 satisfies the algebraic constraints of (1). Usually, if the coefficients of the methods are such that $Y_s = y_1 = \bar{Y}_k$, the best choice for the algebraic component is $z_1 = Z_s$ (or more generally, $z_1 = Z_l$ if $Y_l = y_1$). Alternatively z_1 can be computed as the solution (locally unique provided that (2) is satisfied) of

$$g_y(y_1) f(y_1, z_1) = 0. \tag{8}$$

The existence and uniqueness of the numerical solution given by (6) is not in all cases guaranteed. We will consider two general subclasses of PRK methods for which the scheme (6) has, for sufficiently small h, an unique solution:

- *Type 1*: PRK methods (6) such that $\bar{A}$ is invertible. For this class of methods, only the numerical solution of the differential variables (the y component) is needed to advance one step of the PRK method. It is clear that standard implicit Runge-Kutta methods to solve systems of the form (1) with invertible Runge-Kutta matrix are a particular case of partitioned Runge-Kutta methods (6) of this first type, where $A = \bar{A}$. Half-explicit Runge-Kutta methods studied in [9, 2, 3, 4] are also particular cases of PRK methods (6) of type 1, with A corresponding to an explicit Runge-Kutta method (i.e., is strictly lower triangular), and

$$\begin{pmatrix} A \\ b^T \end{pmatrix} = \begin{pmatrix} 0 \\ \bar{A} \end{pmatrix}. \tag{9}$$

- *Type 2*: PRK methods (6) such that the first row of $\bar{A}$ is null, and $\tilde{A}$ is invertible, where $\tilde{A}$ denotes the matrix obtained from $\bar{A}$ turning its (1,1) entry to 1. For these methods, Z_1 is not determined in (6), and is taken as $Z_1 = z_0$, so that, unlike the methods of type 1, the numerical approximation y_1 does depend on z_0 as well as y_0. The implicit Runge-Kutta methods studied in [12], which includes the Lobatto IIIA methods, fall within this class. The now half-explicit methods proposed in [1] and [13] also belong to this second type of PRK methods. In both cases, A is a strictly lower triangular matrix, and $\bar{A}$ is a lower triangular matrix, such that the sth row of A and the $(s-1)$th row of $\bar{A}$ are equal to the vector b. The methods considered in [1], in addition to these conditions, are constructed in such a way that for every $i \geq 2$ the ith row of $\bar{A}$ coincides with the $(i+1)$th row of A.

It is interesting to note that, when the function g in (1) is linear, the application of a partitioned Runge-Kutta method (6) of type 1 is equivalent to the application of the underlying Runge-Kutta method (that is, the Runge-Kutta method with coefficients a_{ij} and b_i) to the index 1 system (5). This equivalence is also maintained in the case of the application of a partitioned Runge-Kutta method of type 2 with consistent initial values if the parameters b_i and d_i in (6) are such that $y_1 = Y_k$ and $z_1 = Z_k$ for some k.

One may wonder whether PRK methods can be easily generalized for the application to more general index 2 DAE systems of the form

$$y' = f(y,z), \quad 0 = g(y,z), \quad g_z \text{ singular and of constant rank} \tag{10}$$

in a neighborhood of the solution. In that case, certain algebraic variables can be eliminated from the algebraic constraints (see [11], page 477) to transform the original system into Hessenberg form (1) (with different f, g and z). It is known that, for implicit Runge-Kutta methods (of the form (6) with $\bar{A} = A$) of type 1 or 2, the method can be generalized in a straightforward way for systems of the form (10) in such a way that its application is equivalent to the application of the Runge-Kutta method to the transformed system (1). This is possible due to the fact that $\bar{Y}_i = Y_i$ for each i. Unfortunately, this is not the case in the general case of PRK methods. The theoretical analysis of a suitable generalization of method (6) for systems of the form (10) would need special attention, and is not within the scope of this work.

3 Existence and influence of perturbations

The existence and uniqueness for consistent initial values and influence of perturbation for PRK methods of type 1 can be studied in a very similar way to the case of implicit Runge-Kutta methods with invertible matrix A [9, 11]. In the case of methods of type 2, existence of the numerical solution for initial values that do not satisfy (4) must be considered.

Let us denote as $\tilde{A}$ the $s \times s$ matrix whose entries $\tilde{a}_{ij}$ are given by

$$\tilde{a}_{11} = 1, \quad \tilde{a}_{ij} = \bar{a}_{ij} \;\text{ if }\; (i,j) \neq (1,1), \tag{11}$$

and let w_{ij} be the entries of $W = \tilde{A}^{-1}$. In the rest of the section, we will focus our attention to PRK methods of type 2 (i.e. such that the first row of A is null, $Z_1 = z_0$ and $\tilde{A}$ is invertible). However, the results we obtain here can be adapted for PRK methods of type 1, as they can be formally considered as methods of type 2. In fact, just adding an additional stage $Y_0 = \overline{Y}_0 = y_0$, $Z_0 = z_0$ to a s-stage PRK method of type 1, one equivalent PRK method of type 2 with $s+1$ stages is obtained, whose extended $\bar{A}$ matrix is obtained from the original one prepending one null row and one null column.

Lemma 1 *Let us consider the system (1) and (y_0, z_0) such that (3) is satisfied, and assume that $g_y(y)f_z(y,z)$ is invertible in a neighborhood of (y_0, z_0). Then, if $||g_y(y_0)f(y_0,z_0)||$ is sufficiently small, the PRK scheme (6) of type 2 has for $h \le h_0$ a locally unique solution, which smoothly depends on h and (y_0, z_0).*

Note that in this lemma the numerical solution of (6) is only defined for (y_0, z_0) in the manifold $\mathcal{M} = \{(y,z)\ /\ g(y) = 0\}$. If we want to avoid working with functions defined in manifolds, (19) can be extended (following a suggestion of Hairer) to a neighborhood of the manifold replacing in (6) the equations $g(\overline{Y}_i) = 0$ by $g(\overline{Y}_i) = g(y_0)$. A more general result that covers Lemma 1 as well as the extension above is proven below.

Our aim now is to study the influence of perturbations in partitioned Runge-Kutta methods (6) of type 2. Given $(\widehat{y}_0, \widehat{z}_0)$ such that $g(\widehat{y}_0) = \theta_1$, we consider the following scheme

$$
\begin{aligned}
\widehat{Z}_1 &= \widehat{z}_0, \\
i &= 1, \ldots, s, \\
& \qquad \widehat{Y}_i = \widehat{y}_0 + h \sum_{j=1}^{s} a_{ij}(f(\widehat{Y}_j, \widehat{Z}_j) + r_j), \\
& \qquad \widehat{\overline{Y}}_i = \widehat{y}_0 + h \sum_{j=1}^{s} \bar{a}_{ij}(f(\widehat{Y}_j, \widehat{Z}_j) + r_j), \quad g(\widehat{\overline{Y}}_i) = \theta_i \\
\widehat{y}_1 &= \sum_{i=1}^{s} b_i (f(\widehat{Y}_i, \widehat{Z}_i) + r_i), \\
\widehat{z}_1 &= \sum_{i=1}^{s} d_i \widehat{Z}_i.
\end{aligned}
\tag{12}
$$

Let us collect the perturbations in two vectors $r = (r_1, \ldots, r_s)$, $\theta = (\theta_1, \ldots, \theta_s)$. In general, the existence and local uniqueness of the solution of (12) for $\hat{y}_0$ and θ in h-independent neighborhoods is not guaranteed. We formally avoid this defining

$$\delta_i = \frac{\theta_i - \theta_1}{h} = \frac{g(\widehat{\overline{Y}}_i) - g(\widehat{y}_0)}{h}, \quad \delta = (\delta_2, \ldots, \delta_s) \tag{13}$$

(by definition, $\delta_1 = 0$).

Proceeding in a similar way to the proof of Theorem 7.1 of [11] when studying the existence of Runge-Kutta methods with invertible A matrix, the equations $g(\widehat{\overline{Y}}_i) = 0$ in (12) can be replaced by

$$\delta_i = \frac{1}{h}\int_0^1 \frac{d}{d\tau} g(\widehat{y}_0 + \tau(\widehat{\overline{Y}}_i - \widehat{y}_0)) d\tau = \int_0^1 g_y(\widehat{y}_0 + \tau(\widehat{\overline{Y}}_i - \widehat{y}_0)) \sum_{j=1}^{s} \bar{a}_{ij}(f(\widehat{Y}_j, \widehat{Z}_j) + r_j) d\tau.$$

Therefore, replacing $\widehat{\widehat{Y}}_i$ by their explicit expressions, (12) can be expressed in the form

$$F(\widehat{U}, h, \widehat{y}_0, \widehat{z}_0, r, \delta) = 0, \tag{14}$$

where $\widehat{U} = (\widehat{Y}_2, \ldots, \widehat{Y}_s, \widehat{Z}_2, \ldots, \widehat{Z}_s)$ and F is a smooth function.

We want to proof that, for $(\widehat{y}_0, \widehat{z}_0)$ sufficiently close to consistent initial values (y_0, z_0) and sufficiently small r, δ, (12) has for $h \le h_0$ a locally unique solution: First, we see that $F(U^0, 0, y_0, z_0, 0, 0) = 0$, where $U^0 = (y_0, \ldots, y_0, z_0, \ldots, z_0)$. Second, the Jacobian of F with respect to $\widehat{U}$ at $(U^0, 0, y_0, z_0, 0, 0)$ is

$$F_{\widehat{U}}(U^0, 0, y_0, z_0, 0, 0) = \begin{pmatrix} I & 0 \\ \widehat{A} \otimes \partial/\partial y(g_y f)(y_0, z_0) & \widehat{A} \otimes (g_y f_z)(y_0, z_0) \end{pmatrix},$$

where $\widehat{A}$ is the matrix obtained from $\bar{A}$ (or $\tilde{A}$) suppressing its first column and row. This matrix is invertible provided that (2) is satisfied and the matrix $\tilde{A}$ is invertible. It follows from the implicit function theorem that there exists a locally unique solution $\widehat{U} = (\widehat{Y}_2, \ldots, \widehat{Y}_s, \widehat{Z}_2, \ldots, \widehat{Z}_s)$ of (12) which smoothly depends on $(h, \widehat{y}_0, \widehat{z}_0, r, \delta)$. This implies that there exist smooth functions ϕ and φ defined in a neighborhood of $(y_0, z_0, 0, 0, 0)$ such that the solution $(\widehat{y}_1, \widehat{z}_1)$ of the perturbed scheme (12) satisfies

$$\widehat{y}_1 = \widehat{y}_0 + h\phi(\widehat{y}_0, \widehat{z}_0, h, r, \delta), \quad \widehat{z}_1 = \varphi(\widehat{y}_0, \widehat{z}_0, h, r, \delta). \tag{15}$$

Since $\delta_i = (g(\widehat{\widehat{Y}}_i) - g(\widehat{y}_0))/h$, unless the partial derivatives φ_{δ_i} of φ with respect to δ_i satisfy

$$\varphi_{\delta_i}(\widehat{y}_0, \widehat{z}_0, h, r, \delta) = O(h), \quad 2 \le i \le s, \quad \sum_{i=2}^{s} \varphi_{\delta_i}(\widehat{y}_0, \widehat{z}_0, h, r, \delta) = O(h), \tag{16}$$

$\widehat{z}_1$ becomes unstable if θ_i $(1 \le i \le s)$ remains about the same size as $h \to 0$.

It is not difficult to see that the partial derivatives $\partial \widehat{Z}_j^0 / \partial \delta_i$ of $\widehat{Z}_j$ with respect to δ_i evaluated at $(\widehat{y}_0, \widehat{z}_0, h, r, \delta) = (y_0, z_0, 0, 0, 0)$ (so that $\hat{U} = U^0 = (y_0, \ldots, y_0, z_0, \ldots, z_0)$) satisfy

$$g_y(y_0) \sum_{k=1}^{s} \bar{a}_{ik} f_z(y_0, z_0) \frac{\partial \widehat{Z}_k^0}{\partial \delta_j} = \begin{cases} 1 & \text{if} \quad i = j, \\ 0 & \text{else,} \end{cases}$$

and therefore, $\partial \widehat{Z}_j^0 / \partial \delta_i = w_{ji} (g_y f_z)^{-1}(y_0, z_0)$, and

$$\varphi_{\delta_i}(y_0, z_0, 0, 0, 0) = \sum_{j=1}^{s} w_{ji} (g_y f_z)^{-1}(y_0, z_0).$$

Thus, (16) implies that

$$\sum_{j=1}^{s} d_j w_{ji} = 0, \quad 2 \le i \le s, \quad \sum_{i=2}^{s}\sum_{j=1}^{s} d_j w_{ji} = 0,$$

which, by the invertibility of $\tilde{A}$, implies that $d_1 = \cdots = d_s = 0$.

In order to study the influence of the error in the hidden constraint in more detail, the partial derivatives ϕ_z and φ_z of $\phi(y, z, h, r, \delta)$ and $\varphi(y, z, h, r, \delta)$ with respect to z must be analyzed. We first consider the partial derivatives $\partial U^0/\partial \widehat{z}_0$ of $\widehat{U}$ with respect to $\widehat{z}_0$ at $(h, \widehat{y}_0, \widehat{z}_0, r, \delta) = (0, y_0, z_0, 0, 0)$: Clearly, $\partial Y_i^0/\partial \widehat{z}_0 = \partial \overline{Y}_i^0/\partial \widehat{z}_0 = 0$, and from that,

$$(g_y f_z)(y_0, z_0) \sum_{j=1}^{s} \bar{a}_{ij} \partial Z_j^0/\partial \widehat{z}_0 = 0, \quad 2 \le i \le s,$$

which leads to

$$\frac{\partial Z_i^0}{\partial \widehat{z}_0} = w_{i1} I. \tag{17}$$

Then, it is straightforward to check that

$$\phi_z(y_0, z_0, 0, 0, 0) = \left(\sum_{i=1}^{s} b_i w_{i1}\right) f_z(y_0, z_0), \quad \varphi_z(y_0, z_0, 0, 0, 0) = \alpha I, \quad \text{where } \alpha = \sum_{i=1}^{s} d_i w_{i1},$$

If (7) is satisfied, which implies $\sum b_i w_{i1} = 0$, then $\phi_z(y_0, z_0, 0, 0, 0) = 0$, and from the smoothness of ϕ and φ,

$$\begin{aligned} \phi_z(\widehat{y}_0, \widehat{z}_0, h, r, \delta) &= O(h + ||\Delta y_0|| + ||\Delta z_0|| + ||r|| + ||\delta||), \\ \varphi_z(\widehat{y}_0, \widehat{z}_0, h, r, \delta) &= \alpha I + O(h + ||\Delta y_0|| + ||\Delta z_0|| + ||r|| + ||\delta||), \end{aligned}$$

where $\Delta y_i = \widehat{y}_i - y_i$ and $\Delta z_i = \widehat{z}_i - z_i$. In [12] it can be observed (Theorem 4.4) that, in the particular case of $\bar{A} = A$, and under certain conditions on the parameters of the method, the estimate for ϕ_z can be sharpened, obtaining

$$\phi_z(y_0, z_0, h, 0, 0) = O(h^k) \tag{18}$$

for $k > 1$. In Subsection 5.4, we develop a procedure to obtain sufficient conditions on the parameters of the methods for (18) to be satisfied for $k > 1$.

Summing up, we obtain the following result:

Lemma 2 *Let us consider the system (1) and consistent initial values (y_0, z_0) such that (2) is satisfied, and a PRK method (6) of type 2. Then, the perturbed scheme (12) has,* *for* $(\widehat{y}_0, \widehat{z}_0, h, r, \delta)$ *in a neighborhood* $\mathcal{U}$ *of* $(y_0, z_0, 0, 0, 0)$ *(with* δ *defined by (13)), a locally unique solution* $(\widehat{y}_1, \widehat{z}_1, \widehat{Y}_2, \ldots, \widehat{Y}_s, \widehat{Z}_2, \ldots, \widehat{Z}_s)$ *which smoothly depends on* $(\widehat{y}_0, \widehat{z}_0, h, r, \delta)$*. In particular, the perturbed numerical solution* $(\widehat{y}_1, \widehat{z}_1)$ *can be expressed in the form (15), where* ϕ *and* φ *are smooth functions defined in* $\mathcal{U}$*. Furthermore, if* k *is such that (18) is fulfilled, then*

$$\begin{aligned}\Delta y_1 &= (I + O(h))\,\Delta y_0 + \left(h^{k+1} + h||\Delta z_0||\right)\Delta z_0 + h||r|| + ||\theta||,\\ \Delta z_1 &= (\alpha I + O(h) + ||\Delta z_0||)\,\Delta z_0 + ||\Delta y_0|| + ||r|| + \frac{||\theta||}{h},\end{aligned}$$

where $\Delta y_i = \widehat{y}_i - y_i$ *and* $\Delta z_i = \widehat{z}_i - z_i$*.*

4 Convergence

In this section we will consider PRK methods satisfying (7), so that the numerical solution exactly fulfills the algebraic constraints of (1).

According to Lemma 2, the numerical approximations y_n to the solutions $y(t_n)$ of the system (1) at $t_n = t_{n-1} + h_{n-1}$ obtained by means of a PRK method (6) of type 1 or 2 that satisfy (7) can be rewritten as

$$y_{n+1} = y_n + h_n\phi(y_n, z_n, h_n), \quad z_{n+1} = \varphi(y_n, z_n, h_n), \tag{19}$$

where we use the notation $\phi(y, z, h) := \phi(y, z, h, 0, 0)$ and $\varphi(y, z, h) := \varphi(y, z, h, 0, 0)$. This is also true if the alternative way (8) is used to compute the numerical approximations for the z-component.

For PRK methods of type 1, as ϕ and φ do not depend on z_n, the error for the differential component propagates in the same way as for one-step numerical integrators for ODEs, and therefore, its convergence can be studied following the same procedure.

Given (y_0, z_0) satisfying the consistency equations (3)-(4), the local error of the method (19) is defined by

$$\delta^y(y_0, z_0, h) = y(t_0 + h) - y_0 - h\phi(y_0, z_0, h), \tag{20}$$
$$\delta^z(y_0, z_0, h) = z(t_0 + h) - \varphi(y_0, z_0, h). \tag{21}$$

where $(y(t), z(t))$ is the exact solution of (1) with initial values $y(t_0) = y_0, z(t_0) = z_0$.

Theorem 1 *Let us consider the system (1), consistent initial values* (y_0, z_0)*, and a PRK method of type 1 given by (19). Denote* $h = \max h_i$*. If the local errors (20) and (21) satisfy*

$$\delta^y(y, z, h) = O(h^{p+1}), \quad \delta^z(y, z, h) = O(h^m) \tag{22}$$

in a neighborhood of the solution, then, for $nh \leq$ *Constant,*

$$y_n - y(t_n) = O(h^p), \quad z_n - z(t_n) = O(h^{\min(p,m)}).$$

A systematic way of obtaining necessary and sufficient conditions for (22) to be satisfied is developed in Section 5.

The convergence of PRK methods of type 2 cannot be studied in the same way, as the propagation of the error for the algebraic component has to be taken into account. The first proof of optimal convergence results for methods of type 2 appearing in the literature is due to Jay [12], where super-convergence results for certain implicit Runge-Kutta methods ($\bar{A} = A$) of type 2 are obtained. In [1, 13] the convergence of half-explicit PRK methods of type 2 is studied.

The following result, generalization of Lemma 2.9 of [11], will be used in the proof of next theorem:

Lemma 3 *Let* $\{u_n\}$ *and* $\{v_n\}$ *be two sequences of non-negative numbers such that*

$$\begin{aligned} u_{n+1} &\leq (1 + O(h))u_n + O(\varepsilon)v_n + hM, \\ v_{n+1} &\leq O(1)u_n + (\alpha + O(h)v_n + hN, \end{aligned}$$

with $\alpha, M, N \geq 0$*, then, the following estimates hold for sufficiently small* h*,* $\varepsilon \leq ch$*,* $nh \leq Const$*:*

$$\begin{aligned} u_n &\leq C(u_0 + \varepsilon v_0 + M + \varepsilon N), \text{ and} \\ v_n &\leq C(u_0 + (\varepsilon + (\alpha^*)^n)v_0 + M + hN), \quad \text{if } \alpha^* = |\alpha + O(h)| < 1, \\ v_n &\leq C(u_0 + v_0 + M + N), \quad \text{if } |\alpha| = 1. \end{aligned}$$

Proof: It can be proven in a very similar way to Lemma 2.9 of [11], and it is based on the decomposition

$$\begin{pmatrix} 1 + O(h) & O(\epsilon) \\ O(1) & \alpha + O(h) \end{pmatrix} = \begin{pmatrix} 1 & O(\epsilon) \\ O(1) & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 + O(h) & 0 \\ 0 & \alpha + O(h) \end{pmatrix} \begin{pmatrix} 1 & O(\epsilon) \\ O(1) & 1 \end{pmatrix}.$$

□

Theorem 2 *Let us consider the system (1), and the application of a PRK method given by (19), with initial values* (y_0, z_0) *satisfying (3) and* $g_y(y_0)f(y_0, z_0) = O(h^l)$*. Let us denote* $h = \max h_i$*. If* $|\alpha| < 1$*, and (22) and (18) are satisfied in a neighborhood of the solution, then, for* $nh \leq$ *Constant,*

$$y_n - y(t_n) = O(h^{\min(p,m+k,2m,m+l,l+k+1,2l+1)}), \quad z_n - z(t_n) = O(h^{\min(p,m,l)}). \tag{23}$$

Proof: The statement of this theorem can be proven comparing the numerical solution (y_n, z_n) of (19) with the exact solution $(y(t_n), z(t_n))$ of (1) with initial values (y_0, z_0^0), where z_0^0 is the solution of $g_y(y_0)f(y_0, z_0^0) = 0$ which is closest to z_0. Let us denote $\Delta y_n = y_n - y(t_n)$ and $\Delta z_n = z_n - z(t_n)$. The hypothesis of the theorem together with Lemma 2 implies that

$$\begin{pmatrix} \Delta y_{n+1} \\ \Delta z_{n+1} \end{pmatrix} = \begin{pmatrix} I + O(h) & O(h^{k+1} + h||\Delta z_n||) \\ O(1) & \alpha I + O(h + ||\Delta z_n||) \end{pmatrix} \begin{pmatrix} \Delta y_n \\ \Delta z_n \end{pmatrix} - \begin{pmatrix} \delta^y(y(t_n), z(t_n), h_n) \\ \delta^z(y(t_n), z(t_n), h_n) \end{pmatrix}.$$

First, assuming that the errors $||\Delta z_n||$ are sufficiently small so that $\alpha^* = |\alpha + O(h) + \max ||\Delta z_n||| < 1$, Lemma 3 can be applied with $u_n = ||\Delta y_n||$, $v_n = ||\Delta z_n||$, $\varepsilon = h$, α replaced by α^*, $M = O(h^p)$, and $N = O(h^{m-1})$, which implies that $\Delta z_n = O(h^{\min(p,m,l)})$. Second, we again apply Lemma 3 with $u_n = ||\Delta y_n||$, $v_n = ||\Delta z_n||$, $\varepsilon = h^{\min(p,m,l,k)+1}$, $M = O(h^p)$, and $M = O(h^{m-1})$, which gives the estimate for $||\Delta y_n||$. □

Remarks:

1. Lemma 2 guarantees that (18) is fulfilled at least for $k = 1$. In Subsection 5.4, we develop a procedure to obtain in a systematic way sufficient conditions on the coefficients of the methods for (18) to be satisfied for $k > 1$.

2. The application with consistent initial values of a PRK method such that $|\alpha| < 1$ is of order p for the differential variables if (22) and (18) are satisfied with $m \geq k, p-k$. Moreover, if $m > p - k$, the leading term of $y_n - y(t_n)$ is not influenced by the local error of the algebraic component.

3. The estimate for the global error of the z component can be sharpened for $0 < C_1 \leq nh \leq C_2$, obtaining $z_n - z(t_n) = O(h^{\min(p,m,l+k+1,2l+1)})$.

4. In the case of $|\alpha| = 1$, using the similar arguments to those of the proof of the Theorem, it can be proven that

$$y_n - y(t_n) = O(h^{\min(p,m+k,l+k+1,2m-1,2l+1,m+l)}), \quad z_n - z(t_n) = O(h^{\min(p,m-1,l)}).$$

5. In the case of PRK methods of type 1, z_1 can be computed as $z_1 = d_0 z_0 + \sum d_i Z_i$. The global error of the z-component of the application of such a method can be derived considering it as a PRK method of type 2, so that Theorem 2 can be applied with $k = \infty$ and $\alpha = d_0$.

6. If the alternative way (8) of computing the approximation of the algebraic variables is used, then Theorem 2 can still be applied with $m = p + 1$.

5 Order conditions for PRK methods for index 2 DAE systems

In order to verify the order of convergence of a PRK method (6) applied to index 2 systems of the form (1), we need to study, according to Theorems 1 and 2, under which conditions on the parameters of the method is fulfilled (22) for given r and m. In the case of PRK methods of type 2, condition (18) must also be studied.

To verify (22) we need to compare the series expansion in powers of h of the exact solution $(y(t_0+1), z(t_0+h))$ and the numerical solution (y_1, z_1). In [14] we derive the construction of these formal expansions, which turn out to be of the same form as the series obtained by Hairer, Lubich, and Roche in [9] when studying the order condition of implicit Runge-Kutta methods (i.e., PRK methods with $\bar{A} = A$). As in [9], we will use (rooted) trees to represent the independent terms (the *elementary differentials*) of these series expansions.

In Subsection 5.1 we present a general formalism introduced in [14] to deal with series expansions, which will be useful in the rest of this section. The definitions used to expand $(y(t_0+1), z(t_0+h))$ and (y_1, z_1) are given in Subsection 5.2. Subsection 5.3 is devoted to the construction of a set of conditions on the parameters of the method (6) that is equivalent to (22), while in Subsection 5.4, equivalent algebraic conditions are derived for (18).

5.1 Formal series of elementary differentials and elementary operators

Let us consider a numerable set $\mathcal{T}$ of mathematical objects such that each $u \in \mathcal{T}$ has attached a non-negative integer $\rho(u)$, the *order* of u. Assume that there is only an element of $\mathcal{T}$ of order 0, and let us denote it by $\emptyset$.

Let us assume that each $u \in \mathcal{T}$ has associated a function, called *elementary differential* $F(u) : R^N \to R^N$, and that $F(\emptyset)$ is the identity function *id*.

For each $\mathbf{c} : \mathcal{T} \to R$, we denote by $\mathcal{S}(\mathbf{c}, h)$ the formal series

$$\mathcal{S}(\mathbf{c}, h) = \sum_{u \in \mathcal{T}} h^{\rho(u)} \mathbf{c}(u)\, F(u). \tag{24}$$

Definition 1 *Given $u_1, \ldots, u_m \in \mathcal{T} - \{\emptyset\}$, we denote by $X[u_1, \ldots, u_m]$ the linear operator on functions of N variables defined as follows: Given a sufficiently smooth function k of N variables, for each $y \in R^N$,*

$$(X[u_1, \ldots, u_m]k)(y) \quad = \quad \frac{k^{(m)}(y)\,(F(u_1)(y), \ldots, F(u_m)(y))}{\mu_1! \cdots \mu_\nu!}, \tag{25}$$

where $\mu_1, \ldots, \mu_\nu$ are the numbers of mutually equal objects in $u_1, \ldots, u_m$. Clearly, the operator $X[u_1, \ldots, u_m]$ is invariant to permutations of $u_1, \ldots, u_m$. We denote by $X[\emptyset]$ the identity operator.

Definition 2 *Given the set $\mathcal{T}$, we denote by $\widehat{\mathcal{T}}$ the set of unordered m-tuples $[u_1, \ldots, u_m]$ of elements of $\mathcal{T}$,*

$$\widehat{\mathcal{T}} = \{[\emptyset]\} \cup \{[u_1, \ldots, u_m] \ / \ u_1, \ldots, u_m \neq \emptyset\}.$$

Definition 3 *Given $\mathbf{a} : \widehat{\mathcal{T}} \to R$, we denote by $\widehat{\mathcal{S}}(\mathbf{a}, h)$ the formal series of elementary operators*

$$\widehat{\mathcal{S}}(\mathbf{a}, h) = \sum_{[u_1,\ldots,u_m]\in\widehat{\mathcal{T}}} h^{\rho(u_1)+\cdots+\rho(u_m)} \mathbf{a}([u_1, \ldots, u_m])\, X[u_1, \ldots, u_m].$$

The proof of the following result, given in [14], can be easily obtained considering the multivariate Taylor expansion of the function k:

Theorem 3 *If $\mathbf{c} : \mathcal{T} \to R$ with $\mathbf{c}(\emptyset) = 1$, for each smooth function k of N variables*

$$k \circ \mathcal{S}(\mathbf{c}, h) = \widehat{\mathcal{S}}(\mathbf{c}', h)k,$$

where $\mathbf{c}'([u_1, \ldots, u_m]) = \mathbf{c}(u_1) \cdots \mathbf{c}(u_m)$.

5.2 Trees and elementary differentials

Let us consider, given consistent initial values (y_0, z_0) (i.e. satisfying (3)-(4)), the application of one step of the PRK method (6) to the system (1). In [14], the expansions of the numerical solution (y_1, z_1) and the exact solution $(y(t_0 + h), z(t_0 + h))$, together with the expansions of the intermediate values $Y_i, Z_i, \bar{Y}_i$, are studied. There, we systematically derive the set $\mathcal{T}$ and the corresponding elementary differentials $F(u)$ such that formally, following the notation of the previous subsection

$$\begin{pmatrix} y(t_0 + h) \\ z(t_0 + h) \end{pmatrix} = \mathcal{S}(\delta, h)(y_0, z_0), \quad \begin{pmatrix} y_1 \\ z_1 \end{pmatrix} = \mathcal{S}(\mathbf{c}, h)(y_0, z_0), \tag{26}$$

$$\begin{pmatrix} Y_i \\ Z_i \end{pmatrix} = \mathcal{S}(\mathbf{c}_i, h)(y_0, z_0), \quad \bar{Y}_i = \mathcal{S}^1(\bar{\mathbf{c}}_i, h)(y_0, z_0), \tag{27}$$

with suitable coefficients $\delta(u), \mathbf{c}(u), \mathbf{c}_i(u), \bar{\mathbf{c}}_i(u)$. Not surprisingly, these expansions happen to be of the same form as the series obtained by Hairer, Lubich, and Roche [9] when studying the local error of implicit Runge-Kutta methods for index 2 systems of the form (1).

As usual, we will denote by $F(u)$ the elementary differential corresponding to the tree u. Given a vector $x = (y^T, z^T)^T$, we will use the notation $x^1 = y$, $x^2 = z$, and similarly, given $u \in \mathcal{T}$, $\mathbf{a} : \mathcal{T} \to R$,

$$F(u) = \begin{pmatrix} F(u)^1 \\ F(u)^2 \end{pmatrix}, \quad \mathcal{S}(\mathbf{a}, h) = \begin{pmatrix} \mathcal{S}(\mathbf{a}, h)^1 \\ \mathcal{S}(\mathbf{a}, h)^2 \end{pmatrix}.$$

As in [9] (see also [11], Definition VI.8.1), the elements of $\mathcal{T}$ are (rooted) *trees* with two different types of vertices, vertices of type 1 ($\bullet$), and vertices of type 2 ($\circ$). As usual, we write $u = [u_1, \ldots, u_m]_\nu$ ($\nu = 1, 2$) if the root of the tree u is of type ν and $\{u_1, \ldots, u_m\}$ is the collection of trees arising from removing the root of u. For each tree u, its *order* $\rho(u)$ is the number of vertices of type 1 minus the number of vertices of type 2. We will denote by $\emptyset$ the empty tree, with $\rho(\emptyset) = 0$, and $\bullet$ or alternatively $[\emptyset]_1$ the tree with a single vertex of type 1.

Definition 4 *Let us consider the set $\mathcal{T} = \{\emptyset\} \cup \mathcal{T}_1 \cup \mathcal{T}_2$ of such trees recursively defined (as in [9, 11]) as follows:*

1. $\bullet = [\emptyset]_1 \in \mathcal{T}_1$,
2. $[u_1, \ldots, u_m]_1 \in \mathcal{T}_1$ *if* $u_1, \ldots, u_m \in \mathcal{T}_1 \cup \mathcal{T}_2$,
3. $u = [u_1, \ldots, u_m]_2 \in \mathcal{T}_2$ *if* $u_1, \ldots, u_m \in \mathcal{T}_1$ *and* $u \neq [[v]_1]_2$ *with* $v \in \mathcal{T}_2$.

Definition 5 *For each tree u of $\mathcal{T}$, the* elementary differential $F(u)$ *corresponding to u is defined (following the notation of the previous subsection) as follows: $F(\emptyset) = id$, $F(u)^2 = 0$ if $u \in \mathcal{T}_1$, $F(u)^1 = 0$ if $u \in \mathcal{T}_2$, and*

$$\begin{aligned} F(u)^1 &= X[u_1, \ldots, u_m]f, \quad \text{if } u = [u_1, \ldots, u_m]_1 \in \mathcal{T}_1, \\ F(u)^2 &= (-g_y f_z)^{-1} X[u_1, \ldots, u_m]g, \quad \text{if } u = [u_1, \ldots, u_m]_2 \in \mathcal{T}_2. \end{aligned}$$

5.3 Order conditions

Given $\mathbf{a} : \mathcal{T} \to R$, we denote by $\mathbf{a}'$ the mapping $\mathbf{a}' : \mathcal{T} \to R$ such that $\mathbf{a}'(\emptyset) = 0$, and for $\nu = 1, 2$,

$$\mathbf{a}'([u_1, \ldots, u_m]_\nu) = \mathbf{a}'([u_1, \ldots, u_m]) = \mathbf{a}(u_1) \cdots \mathbf{a}(u_m).$$

According to Theorem 3 and Definition 4, it is clear from (1) and (6) that for every tree $u \in \mathcal{T}_1$

$$\begin{aligned} \delta(u) &= \frac{\delta'(u)}{\rho(u)}, \quad \mathbf{c}(u) = \sum_{i=1}^{s} b_i \mathbf{c}'_i(u), \\ \mathbf{c}_i(u) &= \sum_{j=1}^{s} a_{ij} \mathbf{c}'_j(u), \quad \bar{\mathbf{c}}_i(u) = \sum_{j=1}^{s} \bar{a}_{ij} \mathbf{c}'_j(u), \quad 1 \le i \le s. \end{aligned} \tag{28}$$

From (6) it is clear that for each $u \in \mathcal{T}_2$

$$\mathbf{c}(u) = \sum_{i=1}^{s} d_i \mathbf{c}_i(u).$$

As for the coefficients $\delta(u)$ and $\mathbf{c}_i(u)$ for trees $u \in \mathcal{T}_2$, they can be obtained with the help of the following lemma:

Lemma 4 *Given* $\mathbf{a} : \mathcal{T} \to R$ *such that* $g\left(\mathcal{S}(\mathbf{a}, h)(y_0, z_0)\right) = 0$ *for consistent initial values* (y_0, z_0)*, then*

$$\sum_{v \in \mathcal{T}_2} h^{\rho(v)} \mathbf{a}([v]_1) F(v)^2 \quad = \quad \sum_{v \in \mathcal{T}_2} h^{\rho(v)} \mathbf{a}'(v) F(v)^2.$$

Proof: Under the hypothesis of the lemma, Theorem 3 implies that

$$0 = \sum_{[u_1,\dots,u_m] \in \widehat{\mathcal{T}}} h^{\rho(u_1)+\cdots+\rho(u_m)} \mathbf{a}(u_1) \cdots \mathbf{a}(u_m) \, \left(X[u_1,\dots,u_m]g\right)(y_0, z_0).$$

As g does not depend on z, $X[u_1,\dots,u_m]g$ is identically null unless $u_1,\dots,u_m \in \mathcal{T}_1$. Moreover, $X[\emptyset]g = g$ and $X[\bullet]g = g_y f$, and therefore, they are null evaluated at consistent initial values. Thus, under the hypothesis of the lemma,

$$\begin{aligned} 0 \quad &= \sum_{[u_1,\dots,u_m]_2 \in \mathcal{T}_2} h^{\rho(u_1)+\cdots+\rho(u_m)} \mathbf{a}(u_1) \cdots \mathbf{a}(u_m) \, \left(X[u_1,\dots,u_m]g\right)(y_0, z_0) \\ &+ \sum_{v \in \mathcal{T}_2} h^{\rho([v]_1)} \mathbf{a}([v]_1) \, \left(X[[v]_1]g\right)(y_0, z_0). \end{aligned}$$

As $X[[v]_1]g = (g_y f_z) F(v)^2$ and $g_y f_z$ is invertible,

$$\begin{aligned} &\sum_{v \in \mathcal{T}_2} h^{\rho(v)+1} \mathbf{a}([v]_1) \, F(v)^2 (y_0, z_0) \quad = \\ &\qquad \sum_{[u_1,\dots,u_m]_2 \in \mathcal{T}_2} h^{\rho(u_1)+\cdots+\rho(u_m)} \mathbf{a}(u_1) \cdots \mathbf{a}(u_m) \, \Big((-g_y f_z)^{-1} X[u_1,\dots,u_m]g \Big) (y_0, z_0), \end{aligned}$$

which concludes the proof. □

This lemma, together with (28), implies that for each $u \in \mathcal{T}_2$

$$\delta(u) = (\rho(u)+1)\delta'(u), \quad \sum_{j=1}^{s} \bar{a}_{ij} \mathbf{c}_j(u) = \bar{\mathbf{c}}'_i(u), \quad 1 \le i \le s. \tag{29}$$

In the case of methods of type 1 (i.e. with invertible matrix $\bar{A} = (\bar{a}_{ij})$), this implies that

$$\mathbf{c}_i(u) = \sum_{j=1}^{s} w_{ij} \bar{\mathbf{c}}'_j(u), \tag{30}$$

Table 1: Independent order conditions for RK and PRK methods

Order	1	2	3	4	5	6	7
RK	1	1	4	14	56	230	1014
PRK	1	1	5	19	84	381	1856

where the coefficients w_{ij} are the entries of $\bar{A}^{-1}$. For methods of type 2, as $Z_1 = z_0$, and therefore $\mathbf{c}_1(u) = 0$ for every $u \in \mathcal{T}_2$, the second equation of (29) is also true with $\bar{a}_{11}$ replaced by 1, so that (30) is satisfied taking the coefficients w_{ij} as the entries of $\tilde{A}^{-1}$.

Equations (28), (29), and (30) allow us to obtain the coefficients $\delta(u)$, $\mathbf{c}_i(u)$, $\bar{\mathbf{c}}_i(u)$, and $\mathbf{c}(u)$ in a recursive way. Comparing the expansion $\mathcal{S}(\delta, h)$ of the exact solution with that of the numerical solution $\mathcal{S}(\mathbf{c}, h)$, it becomes clear that (22) is fulfilled if the following two conditions are satisfied:

- $\mathbf{c}(u) = \delta(u)$ for all $u \in \mathcal{T}_1$ such that $\rho(u) \leq r$, and
- $\mathbf{c}(u) = \delta(u)$ for all $u \in \mathcal{T}_2$ such that $\rho(u) \leq m - 1$.

Independent order conditions We will next see that not every tree of $\mathcal{T}$ gives rise to an independent order condition for partitioned Runge-Kutta methods. A similar situation arise in the particular case of implicit Runge-Kutta methods for index 2 DAEs (see [11], exercise VI.8.2), but less redundancies in the order conditions occur in the case of general PRK methods. In Table 1, the number of independent order conditions of order up to 7 for the y component of Runge-Kutta methods and partitioned Runge-Kutta methods are compared. In fact, from (28), (29), and (30) it follows that

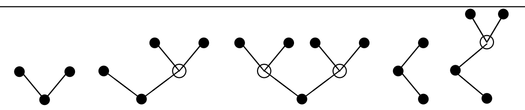
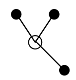
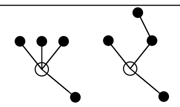
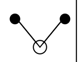
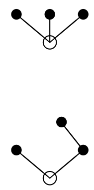
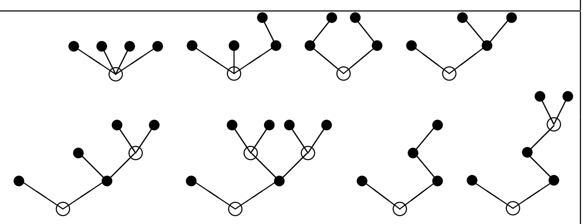
$$\bar{\mathbf{c}}_i([u]_1) = \mathbf{c}'_i(u), \quad \delta([u]_1) = \delta'(u), \quad \text{if } u \in \mathcal{T}_2, \tag{31}$$
$$\mathbf{c}_i([u]_2) = \bar{\mathbf{c}}'_i(u), \quad \delta([u]_2) = \delta'(u), \quad \text{if } u \in \mathcal{T}_1. \tag{32}$$

This implies that only a subset of $\mathcal{T}$ need to be considered to study the order conditions of PRK. Next, we will define three subsets $T_1, \bar{T}_1, T_2$ of $\mathcal{T}$. The trees of $T_1 \subset \mathcal{T}_1$ will be sufficient to study the order of consistency of the intermediate stages Y_i, while the trees of $\bar{T}_1 \subset T_1 \subset \mathcal{T}_1$ will be sufficient for the order of consistency of the values $\bar{Y}_i$. The trees of $T_2 \subset \mathcal{T}_2$ will be related to the order of consistency of the intermediate stages Z_i.

Definition 6 *Let $\bar{T}_1, T_1, T_2 \subset \mathcal{T}$, where $\bar{T}_1 \subset T_1$, be defined recursively as follows:*

1. $\bullet \in \bar{T}_1$,
2. *If $u \in T_1$, then $[u]_1 \in \bar{T}_1$,*

Table 2: Trees of order ≤ 3

Order	1	2	3
$\bar{T}_1$			
$T_1 - \bar{T}_1$			
T_2			

3. *If* $u_1, \ldots, u_m \in T_1 \cup T_2$ *and* $m > 1$*, then* $[u_1, \ldots, u_m]_1 \in \bar{T}_1$*,*

4. *If* $u \in T_2$*, then* $[u]_1 \in T_1 - \bar{T}_1$*,*

5. *If* $u_1, \ldots, u_m \in \bar{T}_1$ *and* $m > 1$*, then* $[u_1, \ldots, u_m]_2 \in T_2$

In Table 2, the set of trees of $T_1 \cup T_2$ up to order 3 are displayed. We are now in conditions to give the main result of this section.

Theorem 4 *Let us consider the application of one step of the PRK method (6) to the system (1) with consistent initial values* $y(t_0) = y_0, z(t_0) = z_0$*. Then, for each* $i = 1, \ldots, s$

1. $\bar{Y}_i - y(t_0 + \bar{c}_i h) = O(h^{q+1})$ *if* $\forall u \in \bar{T}_1$ *of order* $\leq q$, $\bar{\mathbf{c}}_i(u) = \delta(u) \bar{c}_i^{\rho(u)}$,

2. $Y_i - y(t_0 + c_i h) = O(h^{q+1})$ *if* $\forall u \in T_1$ *of order* $\leq q$, $\mathbf{c}_i(u) = \delta(u) c_i^{\rho(u)}$,

3. $Z_i - z(t_0 + c_i h) = O(h^{q+1})$ *if* $\forall w \in T_2 \cup T_1$ *of order* $\leq q$, $\mathbf{c}_i(w) = \delta(w) c_i^{\rho(w)}$,

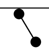
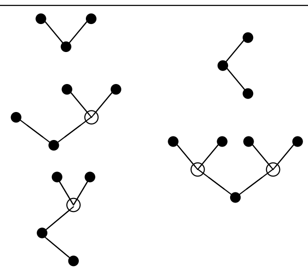
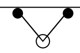
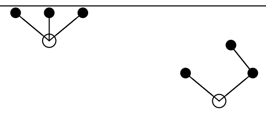
4. $y_1 - y(t_0 + h) = O(h^{r+1})$ *if* $\forall u \in T_1$ *of order* $\leq r$,

$$\sum_{i=1}^{s} b_i \mathbf{c}'_i(u) = \delta(u). \tag{33}$$

5. $z_1 - z(t_0 + h) = O(h^m)$ *if the following two conditions hold*

$$\begin{array}{ll} (a) & \sum_{i=1}^{s} d_i \mathbf{c}_i(u) = \delta(u) \quad \forall u \in T_2 \quad \textit{with} \quad \rho(u) \leq m-1, \\ (b) & \sum_{i=1}^{s} d_i \mathbf{c}'_i(u) = \delta'(u) = \rho(u)\delta(u) \quad \forall u \in T_1 \quad \textit{with} \quad \rho(u) \leq m. \end{array} \tag{34}$$

Table 3: Conditions for $y_1 - y(t_0+h) = O(h^4)$ and $z_1 - z(t_0+h) = O(h^3)$

$\rho(u)$	u	Condition (33)	Condition (34)
1		$\sum b_i = 1$	$\sum d_i = 1$
2		$\sum b_i c_i = 1/2$	$\sum d_i c_i = 1$
3		$\sum b_i c_i^2 = 1/3$	$\sum d_i c_i^2 = 1$
3		$\sum b_i a_{ij} c_j = 1/6$	$\sum d_i a_{ij} c_j = 1/2$
3		$\sum b_i c_i w_{ij} \bar{c}_j^2 = 2/3$	$\sum d_i c_i w_{ij} \bar{c}_j^2 = 2$
3		$\sum b_i (\sum w_{ij} \bar{c}_j^2)^2 = 4/3$	$\sum d_i (\sum w_{ij} \bar{c}_j^2)^2 = 4$
3		$\sum b_i a_{ij} w_{ij} \bar{c}_j^2 = 1/3$	$\sum d_i a_{ij} w_{ij} \bar{c}_j^2 = 1$
1			$\sum d_k w_{k,i} \bar{c}_i^2 = 2$
2			$\sum d_k w_{k,i} \bar{c}_i^3 = 3$
2			$\sum d_k w_{k,i} \bar{c}_i \bar{a}_{ij} c_j = 3/2$

Remarks:

1. Item *3.* implies that, for Z_i having consistency order r, the consistency order of Y_i has to be at least r. This is due to the fact that, according to (32), the coefficients in the expansions of (26) and (27) for $u \in \mathcal{T}_1$ and $[[u]_1]_2$ coincide.

2. Usually, $y_1 = \bar{Y}_k$ for some $k = 1, \ldots, s$, so that it satisfies the constraints of (1). In that case, it is clear that trees u of $T_1 - \bar{T}_1$ need not to be considered in *4*.

3. If $z_1 = Z_k$, $y_1 = Y_k$ for some k (i.e. $d_k = 1$ and $d_i = 0$ for $i \neq k$), and assuming that item *4* is satisfied with $r > m$, only trees of T_2 need to be considered in *5*.

The order conditions (33) and (34) for $r = m = 3$ are displayed in Table 3.

5.4 Additional order conditions for PRK methods of type 2

Given a PRK method (6) of type 2, in order to study its convergence properties applying Theorem 2, in addition to (22), we need to check condition (18). Our aim in this subsection is to develop a systematic procedure to verify (18) in terms of the parameters of the PRK method of type 2.

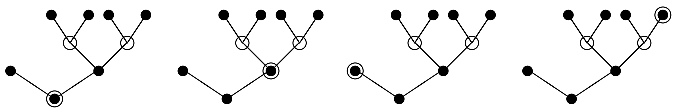


Figure 1: Elements of $\mathcal{DT}$ with same underlying tree of $\mathcal{T}$

In order to do that, the Taylor expansion of $\partial y_1/\partial z_0$ must be analyzed. We will show that formally,

$$\begin{aligned}
\frac{\partial X_i}{\partial z_0} &= \sum_{w\in\mathcal{DT}} h^{\rho(w)}\mathbf{d}_i(w)M(w)(y_0,z_0),\\
\frac{\partial \overline{Y}_i}{\partial z_0} &= \sum_{w\in\mathcal{DT}_1} h^{\rho(w)}\bar{\mathbf{d}}_i(w)M(w)^1(y_0,z_0),\\
\frac{\partial y_1}{\partial z_0} &= \sum_{w\in\mathcal{DT}_1} h^{\rho(w)}\mathbf{d}(w)M(w)^1(y_0,z_0),
\end{aligned} \tag{35}$$

where we denote

$$X_i = \begin{pmatrix} Y_i \\ Z_i \end{pmatrix}, \quad M(w) = \begin{pmatrix} M(w)^1 \\ M(w)^2 \end{pmatrix},$$

$\mathcal{DT} = \mathcal{DT}_1 \cup \mathcal{DT}_2$ is a certain set of mathematical objects related to the trees of $\mathcal{T}$ as we describe below, the $M(w)$ are matrix valued functions that only depend on w and the system (1) to be integrated, $\rho(w)$ is a non-negative integer (the *order of* w), and the coefficients $\mathbf{d}(w), \mathbf{d}_i(w), \bar{\mathbf{d}}_i(w)$ only depend on w and the parameters of the method.

The elements of $\mathcal{DT}_\nu$ ($\nu = 1, 2$) can be represented as trees of $\mathcal{T}_\nu$ where one of the vertices of type 1 ($\bullet$) has been highlighted. The order of such a $w \in \mathcal{DT}$ is the order of the underlying tree of $\mathcal{T}$. We consider that the empty tree gives rise to an element of $\mathcal{DT}_2$ of order 0. Figure 1 shows all the different elements of $\mathcal{DT}$ with a particular underlying tree of $\mathcal{T}$ (the highlighted vertex of type 1 is represented by $\odot$).

In order to get a rigorous recursive definition of $\mathcal{DT}, \mathcal{DT}_1, \mathcal{DT}_2$ we decompose each $w \in \mathcal{DT}$ of order ≥ 1 in a unique way as follows: We denote by $(\emptyset)$ the element of $\mathcal{DT}_2$ whose underlying tree of $\mathcal{T}$ is $\emptyset$. If the highlighted vertex of $w \in \mathcal{DT}$ is the root of the underlying tree $v \in \mathcal{T}$, then w is decomposed as $w = (v, (\emptyset))$. As for the rest of the $w \in \mathcal{DT}$, in analogous way to the trees of $\mathcal{T}$, they can be represented as $w = [v_1, \ldots, v_m, w']_\nu$ ($\nu = 1, 2$), where w' is the subtree with the highlighted vertex of type 1. In that case, w is decomposed as $w = (v, w')$, where $v = [v_1, \ldots, v_m]_\nu$. Note that all possible v of such decompositions belongs to $\mathcal{T}^* = \mathcal{T}_1 \cup \mathcal{T}_2^*$, where

$$\mathcal{T}_2^* = \{[v_1, \ldots, v_m]_2 \ / \ v_1, \ldots, v_m \in \mathcal{T}_1\} \cup \{\circ\} = \mathcal{T}_2 \cup \{[[v]_1]_2 \ / \ v \in \mathcal{T}_2\} \cup \{[\bullet]_2\} \cup \{\circ\}.$$

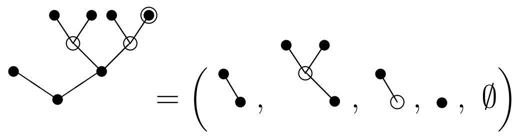


Figure 2: Element of $\mathcal{DT}$ represented as an m-tuple

In analogous way to $\bullet = [\emptyset]_1$, we denote as $\circ$ or $[\emptyset]_2$ the tree with a single vertex of type 2.

Definition 7 *Let $\mathcal{DT}_1, \mathcal{DT}_2$ the sets defined recursively as follows:*

1. $(\emptyset) \in \mathcal{DT}_2$,
2. $(v, w) \in \mathcal{DT}_1$ *if* $v \in \mathcal{T}_1$ *and* $w \in \mathcal{DT}_1 \cup \mathcal{DT}_2$,
3. $(v, w) \in \mathcal{DT}_2$ *if* $v \in \mathcal{T}_2$, $w \in \mathcal{DT}_1$, *and* $(v, w) \neq (\circ, (\bullet, w'))$ *with* $w' \in \mathcal{DT}_2$.

Note that with this decomposition of the elements of $\mathcal{DT} = \mathcal{DT}_1 \cup \mathcal{DT}_2$, they can be represented in a unique way as m-tuples ($m \geq 1$) of the form $(v_1, \ldots, v_{m-1}, \emptyset)$, where $v_1, \ldots, v_{m-1} \in \mathcal{T}^*$ and $v_1 \cdot (v_2 \cdots (v_{m-2} \cdot v_{m-1}) \cdots)$ is a tree of $\mathcal{T}$ (its underlying tree), and the highlighted vertex corresponds to the root of v_{m-1} (and therefore v_{m-1} must belong to $\mathcal{T}_1$).

An example of decomposition of elements of $\mathcal{DT}$ is displayed in Figure 2.

Definition 8 *For each $v \in \mathcal{T}^* \cup \{\emptyset\}$, we define the matrix valued function $F^*(v) = (F^*(w)^{1T}, F^*(w)^{2T})^T$ as follows: $F^*(\emptyset)^1 = 0$, $F^*(\emptyset)^2 = I$, $F^*(v)^2 = 0$ if $v \in \mathcal{T}_1$, $F^*(v)^1 = 0$ if $v \in \mathcal{T}_2^*$, and*

$$
\begin{aligned}
F^*(v)^1 &= X[v_1, \ldots, v_m] f', \quad \text{if } u = [v_1, \ldots, v_m]_1 \in \mathcal{T}_1, \\
F^*(v)^2 &= (-g_y f_z)^{-1} X[v_1, \ldots, v_m] g_y, \quad \text{if } u = [v_1, \ldots, v_m]_2 \in \mathcal{T}_2^*.
\end{aligned}
$$

Definition 9 *For each $w \in \mathcal{DT}$, we define the matrix valued function $M(w)$ such that $M(\emptyset) = F^*(\emptyset)$, and*

$$
\begin{aligned}
M(w)(y, z) &= F^*(v)(y, z) M(w')(y, z), \quad \text{if } w = (v, w') \in \mathcal{DT}_1, \\
M(w)(y, z) &= F^*(v)(y, z) M(w')^1(y, z), \quad \text{if } w = (v, w') \in \mathcal{DT}_2.
\end{aligned}
$$

Theorem 5 *Let us consider the application of a step of a PRK method (6) of type 2 to the system (1) with consistent initial values (y_0, z_0), and denote $X_i = (Y_i^T, Z_i^T)^T$. Then,* *the partial derivatives with respect to* z_0 *of* X_i, $\overline{Y}_i$, *and* y_1 *formally satisfy (35), where the coefficients* $\mathbf{d}_i(w), \bar{\mathbf{d}}_i(w), \mathbf{d}(w)$ *can be recursively obtained as follows:* $\mathbf{d}_i(\emptyset) = w_{i1}$, *and*

$$\begin{aligned}
\mathbf{d}_i(w) &= \sum_{j=1}^{s} a_{ij}\mathbf{d}'_j(w), \quad \textit{if } w \in \mathcal{DT}_1, \\
\bar{\mathbf{d}}_i(w) &= \sum_{j=1}^{s} \bar{a}_{ij}\mathbf{d}'_j(w), \quad \textit{if } w \in \mathcal{DT}_1, \\
\mathbf{d}_i(w) &= \sum_{j=1}^{s} w_{ij}\bar{\mathbf{d}}'_j(w), \quad \textit{if } w \in \mathcal{DT}_2, \\
\mathbf{d}(w) &= \sum_{j=1}^{s} b_i\mathbf{d}'_i(w), \quad \textit{if } w \in \mathcal{DT}_1,
\end{aligned}$$

where for each $w = (v, w') \in \mathcal{DT}$

$$\mathbf{d}'_i(w) = \mathbf{c}'_i(v)\mathbf{d}_i(w'), \quad \mathbf{d}'_i(w) = \bar{\mathbf{c}}'_i(v)\bar{\mathbf{d}}_i(w').$$

Proof: From (6) we obtain that

$$\begin{aligned}
\frac{\partial y_1}{\partial z_0} &= h\sum_{i=1}^{s} b_i F'(X_i)\frac{\partial X_i}{\partial z_0}, \\
\frac{\partial Y_i}{\partial z_0} &= h\sum_{j=1}^{s} a_{ij} F'(X_j)\frac{\partial X_j}{\partial z_0}, \\
\frac{\partial \bar{Y}_i}{\partial z_0} &= h\sum_{j=1}^{s} \bar{a}_{ij} F'(X_j)\frac{\partial X_j}{\partial z_0}, \quad 0 \;=\; g_y(\bar{Y}_i)\frac{\partial \bar{Y}_i}{\partial z_0}.
\end{aligned} \tag{36}$$

We know from Lemma 2 that the partial derivatives with respect to z_0 of $y_1, \bar{Y}_i, Y_i, Z_i$ are locally unique, and are determined by (36). It is then sufficient to prove that (36) formally holds replacing the partial derivatives according to (35).

Theorem 3 together with (27) implies that formally

$$\begin{aligned}
hf'(X_i) &= h\sum_{[u_1,\ldots,u_m]\in\widehat{\mathcal{T}}} h^{\rho(u_1)+\cdots+\rho(u_m)}\,\mathbf{c}'_i([u_1,\ldots,u_m])\,(X[u_1,\ldots,u_m]f')(y_0,z_0) \\
&= \sum_{u\in\mathcal{T}_1} h^{\rho(u)}\,\mathbf{c}'_i(u)\,F^*(u)^1(y_0,z_0), \\
g_y(\bar{Y}_i) &= \sum_{\substack{[u_1,\ldots,u_m]\in\widehat{\mathcal{T}} \\ u_l\in\mathcal{T}_1}} h^{\rho(u_1)+\cdots+\rho(u_m)}\,\bar{\mathbf{c}}'_i([u_1,\ldots,u_m])\,(X[u_1,\ldots,u_m]g_y)(y_0,z_0) \\
&= (-g_yf_z)(y_0,z_0)\sum_{u\in\mathcal{T}_2^*} h^{\rho(u)+1}\,\bar{\mathbf{c}}'_i(u)\,F^*(u)^2 y_0,z_0).
\end{aligned}$$

These equalities, (35), (36), and the Definition 7 lead to

$$\begin{aligned}\frac{\partial Y_i}{\partial z_0} &= \sum_{v\in\mathcal{T}_1}\sum_{w'\in\mathcal{DT}} h^{\rho(v)+\rho(w')}\sum_{j=1}^{s} a_{ij}c_j'(v)\mathbf{d}_j(w')\,F^*(v)^1M(w')(y_0,z_0)\\ &= \sum_{w\in\mathcal{DT}_1} h^{\rho(w)}\sum_{j=1}^{s} a_{ij}\mathbf{d}_j'(w)M(w)^1(y_0,z_0).\end{aligned}$$

In a similar way, one can obtain

$$\begin{aligned}\frac{\partial \bar{Y}_i}{\partial z_0} &= \sum_{w\in\mathcal{DT}_1} h^{\rho(w)}\sum_{j=1}^{s} \bar{a}_{ij}\mathbf{d}_j'(w)M(w)^1(y_0,z_0),\\ \frac{\partial y_1}{\partial z_0} &= \sum_{w\in\mathcal{DT}_1} h^{\rho(w)}\sum_{i=1}^{s} b_i\mathbf{d}_i'(w)M(w)^1(y_0,z_0).\end{aligned}$$

Thus, the first three equalities of (36) are satisfied. As for the last one, with similar arguments, taking into account the invertibility of $(g_yf_z)(y_0,z_0)$, the following can be obtained

$$\begin{aligned}0 &= h\sum_{v\in\mathcal{T}_2^*}\sum_{w'\in\mathcal{DT}_1} h^{\rho(v)+\rho(w')}\bar{\mathbf{c}}_i'(v)\bar{\mathbf{d}}_i(w')\,F^*(v)^2M(w')^1(y_0,z_0)\\ &= h\sum_{w\in\mathcal{DT}_2} h^{\rho(w)}\bar{\mathbf{d}}_i'(w)M(w)^2(y_0,z_0)\\ &+ h\sum_{w\in\mathcal{DT}_2} h^{\rho(w)}\bar{\mathbf{c}}_i'(\circ)\bar{\mathbf{d}}_i(\bullet,w)F^*(\circ)^2M(\bullet,w)^1(y_0,z_0).\end{aligned}$$

Taking into account that for $w\in\mathcal{DT}_2$

$$\bar{\mathbf{d}}_i'(\bullet,w)=\sum_{j=1}^{s}\bar{a}_{ij}\bar{\mathbf{c}}_j'(\bullet)\mathbf{d}_j(w)=\sum_{j=1}^{s}\bar{a}_{ij}\bar{\mathbf{d}}_j(w),$$

$\bar{\mathbf{c}}_i'(\circ)=\bar{\mathbf{c}}_i'([\emptyset])=1$, $F^*(\circ)^2M(\bullet,w)^1=-M(w)^2$, $\partial Z_1/\partial z_0=I$, and the definition of the coefficients w_{ij}, the last equality of (36) can be obtained. □

Now, the main result of this subsection follows:

Theorem 6 *Let us consider a PRK method (6) of type 2 given in the form (19). Condition (18) is satisfied if*

$$\mathbf{d}(w)=0 \quad \textit{for each } w\in\mathcal{DT}_1 \quad \textit{of order } \le k. \tag{37}$$

The only element of order 1 of $\mathcal{DT}_1$ is $(\bullet,\emptyset)$, so that (18) is satisfied for $k=1$ if

$$0=\mathbf{d}(\bullet,\emptyset)=\sum_{i=1}^{s} b_i\mathbf{c}_i'(\bullet)\mathbf{d}(\emptyset)=\sum_{i=1}^{s} b_iw_{i1}. \tag{38}$$

This equality is automatically fulfilled if the PRK method is such that (7) is satisfied, so that in that case (18) is satisfied at least for $k = 1$, as we already proven in Section 3.

It is interesting to note that not all of the elements of $\mathcal{DT}$ give rise to independent conditions of the form (37): The conditions corresponding to elements of $\mathcal{DT}$ of the form $(u_1, \ldots, u_m, \bullet, \emptyset)$ where the root of u_m is of type 2 (for instance, that of Figure 2) are also automatically fulfilled (even if (7) is not satisfied). Moreover, redundancies similar to those appearing for the order conditions studied in the previous subsection appear due to (31)-(32).

Now, it is a straightforward matter to get algebraic conditions on the parameter of the method (6) that guarantee (18) for $k = 2$. The only trees of $\mathcal{T}_1$ of order 2 are $[\bullet]_1$ and $[[\bullet, \bullet]_2]_1$, and therefore, there are four elements of order 2 in $\mathcal{DT}_1$: $([\bullet]_1, \emptyset)$, $(\bullet, \bullet, \emptyset)$, $([[\bullet, \bullet]_2]_1, \emptyset)$, and $(\bullet, [\bullet]_2, \bullet, \emptyset)$. The coefficient of the last one is identically null, and from the rest, we get

$$\sum_{i=1}^{s} b_i c_i w_{i1} = 0, \quad \sum_{i,j=1}^{s} b_i a_{ij} w_{j1} = 0, \quad \sum_{i,j=1}^{s} b_i w_{ij} \bar{c}_j^2 w_{i1} = 0. \tag{39}$$

Hence, if in addition to (7) (or at least (38)) the PRK method (6) satisfies condition (39), then (18) is fulfilled for $k = 2$.

6 Construction of PRK methods. Simplifying assumptions

Here, we will focus our attention to the construction of PRK methods which satisfy (7).

6.1 Basic simplifying assumptions

Let us consider the following simplifying assumptions:

$$\begin{aligned} C(q):& \quad \sum_{j=1}^{s} a_{ij} c_j^{l-1} &=& \frac{c_i^l}{l}, \quad 1 \le i \le s, \quad 1 \le l \le q, \\ \bar{C}(\bar{q}):& \quad \sum_{j=1}^{s} \bar{a}_{ij} c_j^{l-1} &=& \frac{\bar{c}_i^l}{l}, \quad 1 \le i \le s, \quad 1 \le l \le \bar{q}. \end{aligned}$$

For PRK methods of type 1 and type 2, condition $\bar{C}(\bar{q})$ is equivalent to

$$I\bar{C}(\bar{q}): \quad \sum_{j=1}^{s} w_{ij} \bar{c}_j^l \; = \; l c_i^{l-1}, \quad 1 \le i \le s, \quad 1 \le l \le \bar{q},$$

where the coefficients w_{ij} are the entries of $\bar{A}^{-1}$ for methods of type 1, and the entries of $\tilde{A}^{-1}$ for methods of type 2.

Using Theorem 4 it is not difficult to prove the following result:

Lemma 5 *Given a PRK method of type 1 or 2, if $C(q)$ and $\bar{C}(\bar{q})$ are fulfilled, then,*

$$\begin{aligned} Y_i - y(t_0 + c_i h) &= O(h^{\min(q,\bar{q})+1}), \quad Z_i - z(t_0 + c_i h) \;=\; O(h^{q^*}), \\ \overline{Y}_i - y(t_0 + \bar{c}_i h) &= O(h^{q^*+1}) \end{aligned}$$

for $i = 1, \dots, s$, where $q^* = \min(q+1, \bar{q})$. This implies that the order conditions corresponding to trees with some subtree u satisfying one of the following conditions are redundant:

1. *$u \in T_2$ and $\rho(u) < q^*$,*
2. *$u \in T_1$ and $\rho(u) \leq \min(q, \bar{q})$,*
3. *$u \in \bar{T}_1$, it is attached to a vertex of type 2, and $\rho(u) \leq q^*$.*

6.2 Partitioned collocation methods

An interesting subclass of implicit PRK methods can be obtained generalizing the RK methods for index 2 DAEs constructed as collocation methods (Definition VI.7.7 of [11]).

Definition 10 *Let $\{c_1, \dots, c_s\}$ and $\{\bar{c}_1, \dots, \bar{c}_s\}$ be two sets of s distinct real numbers, and denote by $u(t), v(t)$ the polynomials of degree s which satisfy*

$$\begin{aligned} u(t_0) &= y_0, \quad v(t_0) = z_0, \\ u'(t_0 + c_i h) &= f(u(t_0 + c_i h), v(t_0 + c_i h)), \quad 1 \leq i \leq s, \\ 0 &= g(u(t_0 + \bar{c}_i h)), \quad 1 \leq i \leq s. \end{aligned} \tag{40}$$

The numerical solution at $t = t_0 + h$ given by the corresponding partitioned collocation method *is*

$$y_1 = u(t_0 + h), \quad z_1 = v(t_0 + h).$$

It is not difficult to see that this numerical solution is equivalent to a s-stage PRK method (6) that satisfies $C(s)$ and $\bar{C}(\bar{s})$. It is natural to consider partitioned collocation methods with $\bar{c}_s = 1$, so that $g(y_1) = 0$ (i.e., the equivalent PRK method satisfies (7)). If $\bar{c}_i \neq 0$ for all i, it is a PRK method of type 1, and of type 2 otherwise. Well known particular cases of these partitioned collocation methods are the (non partitioned) collocation methods, where $\bar{c}_i = c_i$, for instance, the Radau IIA (type 1), and Lobatto IIIA (type 2) [11, 12].

Next, we present a result that will allow the construction of an interesting family of partitioned collocation methods that does not fall within the family of (non partitioned) Runge-Kutta methods:

Theorem 7 *If $\bar{c}_s = 1$ and $\bar{c}_i \neq 0$ for all i, then, the local error for the y-component of the partitioned collocation method (40) satisfies*

$$y_1 - y(t_0 + h) = O(h^{\min(p,\bar{p})+1}), \tag{41}$$

where p is the order of the quadrature formula corresponding to the s nodes $c_1, \ldots, c_s$ (and weights $b_i = \bar{a}_{si}$), and $\bar{p}$ is the order of the quadrature formula of the $s+1$ nodes $\bar{c}_0 = 0, \bar{c}_1, \ldots, \bar{c}_s = 1$.

Furthermore,

$$u(t) - y(t) = O(h^{s+1}), \quad v(t) - z(t) = O(h^s), \quad t_0 \leq t \leq t_0 + h. \tag{42}$$

Proof: This result can be proven slightly modifying the proofs of Theorem VI.7.8 and VI.7.9 of [11]:

First, following the proof of Theorem VI.7.8, (42) and the boundedness of the derivatives of $(u(t), v(t))$ are proven using Lemma 5 and the fact that $C(s)$ and $\bar{C}(s)$ are satisfied. Second, as in the proof of Theorem VI.7.9, $\delta(t)$ and $\theta(t)$ are defined by

$$\begin{aligned} u'(t) &= f(u(t), v(t)) + \delta(t), \\ 0 &= g(u(t)) + \theta(t), \end{aligned}$$

and an identity of the form

$$u(t_0 + h) - y(t_0 + h) = \int_{t_0}^{t_0+h} S_1(t_0 + h, t)\delta(t)dt - \int_{t_0}^{t_0+h} \frac{\partial}{\partial t} S_1(t_0 + h, t)\theta(t)dt,$$

can be proven.

By definition of $\delta(t)$ and $\theta(t)$, $\delta(t_0 + c_i h) = 0$ for $i = 1, \ldots, s$ and $\theta(t_0 + \bar{c}_i h) = 0$ for $i = 0, 1, \ldots, s$. Thus, (41) can be obtained applying the quadrature formula corresponding to the nodes $c_1, \ldots, c_s$ to approximate the integral involving $\delta(t)$, and using the quadrature formula with nodes $\bar{c}_0 = 0, \bar{c}_1, \ldots, \bar{c}_s$ to integrate the integral involving $\theta(t)$. $\Box$

Gauss-Lobatto methods Given the number of stages s, let us consider the $2s$th order Gaussian quadrature nodes $c_1 < \cdots < c_s$, that is, the zeros of the shifted Legendre polynomial of degree s

$$P_s(x) = \frac{d^s}{dx^s} \left(x^s (x-1)^s \right),$$

and the $2s$th Lobatto quadrature nodes $0 = \bar{c}_0 < \bar{c}_1 < \ldots < \bar{c}_s = 1$, i.e. the zeros of the polynomial of degree $s+1$

$$\int_0^x P_s(\tau) d\tau = \frac{d^{s-1}}{dx^{s-1}} \left(x^s (x-1)^s \right).$$

Table 4: 2-stage Gauss-Lobatto PRK method

$$
\begin{array}{c|cc}
\frac{3-\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\
\frac{3+\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
\qquad
\begin{array}{c|cc}
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\
1 & \frac{1}{2} & \frac{1}{2} \\
\hline
 & &
\end{array}
$$

According to Theorem 7 and 1, the corresponding PRK method (of type 1) has order of convergence $2s$ for the y component.

Furthermore, the following orthogonality condition is satisfied ($1 \le i \le s$)

$$0 = \int_0^{\bar{c}_i} P_s(x)dx = \int_0^{\bar{c}_i} (x-c_1)\cdots(x-c_s)dx,$$

which implies that $\bar{C}(s+1)$ is satisfied, and therefore, $\overline{Y}_i - y(t_0+\bar{c}_i h) = O(h^{s+2})$ and $Z_i - z(t_0+c_i h) = O(h^{s+1})$. This makes possible to obtain, using internal stages of the previous step, dense output of global order $O(h^{s+2})$ for $y(t)$ (respectively $O(h^{s+1})$ for $z(t)$), interpolating for the internal stages $\overline{Y}_i$ (resp. Z_i) of the current step (including $y_0 = \overline{Y}_0$) and one additional internal stage $\overline{Y}_{s-1}$ (Z_s) of the previous step.

As the underlying Runge-Kutta methods are collocation methods based of the Gaussian quadratures (the Kuntzmann-Butcher methods), one can expect that their good stability properties are inherited (at least when g is linear) by these new PRK methods. Moreover, it is easy to check from (40) and the symmetry of the Gauss and Lobatto quadrature formulas that these partitioned collocation methods are symmetric.

In particular, it is not difficult to see that the Gauss-Lobatto PRK method of one stage is a natural generalization to index 2 DAEs (1) of the implicit midpoint method for ODEs, that is

$$y_1 = y_0 + hf\left(\frac{y_0+y_1}{2}, \frac{z_0+z_1}{2}\right), \quad g(y_1)=0.$$

More examples of these Gauss-Lobatto methods are given in Tables 4 and 5. For each method, two Butcher tableaux are displayed,

$$\begin{array}{c|c} c & A \\ \hline & b \end{array}, \quad \text{and} \quad \begin{array}{c|c} \bar{c} & \bar{A} \\ \hline & \end{array}.$$

Table 5: 3-stage Gauss-Lobatto PRK method

$\frac{5-\sqrt{15}}{10}$	$\frac{5}{36}$	$\frac{2}{9} - \frac{\sqrt{15}}{15}$	$\frac{5}{36} - \frac{\sqrt{15}}{30}$
$\frac{1}{2}$	$\frac{5}{36} + \frac{\sqrt{15}}{24}$	$\frac{2}{9}$	$\frac{5}{36} - \frac{\sqrt{15}}{24}$
$\frac{5-\sqrt{15}}{10}$	$\frac{5}{36} + \frac{\sqrt{15}}{30}$	$\frac{2}{9} + \frac{\sqrt{15}}{15}$	$\frac{5}{36}$
	$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

$\frac{5-\sqrt{5}}{10}$	$\frac{25-\sqrt{5}+6\sqrt{15}}{180}$	$\frac{10-4\sqrt{5}}{45}$	$\frac{25-\sqrt{5}-6\sqrt{15}}{180}$
$\frac{5+\sqrt{5}}{10}$	$\frac{25+\sqrt{5}+6\sqrt{15}}{180}$	$\frac{10+4\sqrt{5}}{45}$	$\frac{25+\sqrt{5}-6\sqrt{15}}{180}$
1	$\frac{5}{18}$	$\frac{4}{9}$	$\frac{5}{18}$

6.3 Implicit PRK methods of type 1

In principle, there can exist interesting implicit PRK methods that are not partitioned collocation methods. The following result, which generalizes Theorem 5.9 of [9] can be used to construct implicit PRK methods of high order:

Theorem 8 *Given a PRK method (6) of type 1 such that (7) is satisfied, if there exist* $\bar{b}_1, \ldots, \bar{b}_s$ *such that, in addition to* $C(q)$ *and* $\bar{C}(\bar{q})$*, the following simplifying assumptions are fulfilled:*

$$
\begin{aligned}
B(p):& \quad \sum_{i=1}^{s} b_i c_i^{l-1} = \frac{1}{l}, \quad l = 1, \ldots, p; \\
\bar{B}(\bar{p}):& \quad \sum_{i=1}^{s} \bar{b}_i \bar{c}_i^{l-1} = \frac{1}{l}, \quad l = 1, \ldots, \bar{p}; \\
D(r):& \quad \sum_{j=1}^{s} b_j c_j^{l-1} a_{ji} = b_i(1 - c_i^l), \quad i = 1, \ldots, s, \quad l = 1, \ldots, r; \\
\bar{D}(\bar{r}):& \quad \sum_{j=1}^{s} \bar{b}_j \bar{c}_j^{l-1} \bar{a}_{ji} = b_i(1 - c_i^l), \quad i = 1, \ldots, s, \quad l = 1, \ldots, \bar{r};
\end{aligned}
$$

then, the local error for the y*-component of the PRK method satisfies* $y_1 - y(t_0 + h) = O(h^{R+1})$*, where*

$$
R = \min(p, \bar{p}, 2q + 2, 2\bar{q}, r + q + 1, r + \bar{q} + 1, \bar{r} + q + 2, \bar{r} + \bar{q} + 1). \tag{43}
$$

Remarks:

1. In the particular case of Runge-Kutta methods, as $\bar{c} = c$, $\bar{b} = b$, and $\bar{A} = A$, we have that $\bar{p} = p$, $\bar{r} = r$, $\bar{q} = q$, and therefore $R = \min(p, 2q, r + q + 1)$, as stated in Theorem 5.9 of [9].

2. Multiplying both sides of the equality of $\bar{D}(\bar{r})$ by w_{ik} and extending the sum over $i = 1 \ldots, s$, the following equivalent condition is obtained:

$$I\bar{D}(\bar{r}): \qquad \sum_{i=1}^{s} b_i(1-c_i^l)w_{ij} = \bar{b}_j \bar{c}_j^{l-1}, \quad i = j, \ldots, s, \quad l = 1, \ldots, \bar{r}.$$

3. Note that condition $I\bar{D}(1)$ uniquely determine the $\bar{b}_i$ coefficients in terms of the parameters of the method.

Proof of Theorem 8: We already saw in Lemma 5 how $C(q)$ and $\bar{C}(\bar{q})$ simplify the order conditions. To describe the effect of the rest of the simplifying assumptions, we will use the Butcher notation: given $v, w_1, \ldots, w_k \in \mathcal{T}$, $\nu = 1, 2$, $r \geq 1$

$$[v^l, w_1, \ldots, w_k]_\nu = [\overbrace{v, \ldots, v}^{l}, w_1, \ldots, w_k]_\nu.$$

It is not difficult to see that

- $B(p)$ implies that the order conditions for the trees $\bullet$ and the 'bushy' trees $[\bullet^{l-1}]_1$ $(1 \leq l \leq p)$ are satisfied.
- The condition $\bar{B}(\bar{p})$ correspond, provided that $\bar{D}(1)$ is satisfied, to the order conditions of the trees $[\bullet, [\bullet^{l-1}]_2]_1$ $(1 \leq l \leq p)$.
- Condition $D(r)$ makes redundant the order conditions for trees of T_1 of the form $[\bullet^{l-1}, [u_1, \ldots, u_m]_1]_1$, for $l = 1, \ldots, r$.
- $\bar{D}(\bar{r})$ (which is equivalent to $I\bar{D}(\bar{r})$) implies that the order conditions for trees of T_1 of the form $[\bullet^l, [u_1, \ldots, u_m]_2]_1$ $(2 \leq l \leq \bar{r})$ and $[\bullet, [\bullet^{l-1}, [u_1, \ldots, u_m]_1]_2]_1$ $(1 \leq l \leq \bar{r})$ are redundant.

Taking into account this and Lemma 5, it can be seen that the trees of $\bar{T}_1$ with minimal order whose order conditions are not assured to be satisfied by the hypothesis of the theorem are: $[\bullet^p]_1$, $[\bullet, [\bullet^{\bar{p}}]_2]_1$, $[u, v]_1$ with $\rho(u), \rho(v) = q^* = \min(q+1, \bar{q})$, $[\bullet^{\bar{r}+1}, [\bullet^{q^*+1}]_2]_1$, $[\bullet, [\bullet^{\bar{r}}, [\bullet^{\bar{q}}]_1]_2]_1$, and $[\bullet^r, u]$ with $u \in T_1$ such that $\rho(u) = \min(q, \bar{q}) + 1$. This leads to the statement of the theorem. $\Box$

The following result, similar to Lemma IV.5.4 of [11], is useful, together with the referred lemma and Theorem 8, in the construction of different implicit PRK methods of high order.

Lemma 6 *Given a PRK method (6),*

1. $\bar{C}(\bar{q}), \bar{D}(\bar{r}), B(\bar{q}+\bar{r}) \Rightarrow \bar{B}(\bar{q}+\bar{r})$.

2. If $\bar{c}_1, \ldots, \bar{c}_s$ are distinct and non null, then

$$\bar{C}(s), B(s+\bar{r}), \bar{B}(s+\bar{r}) \Rightarrow \bar{D}(\bar{r}).$$

3. If $\bar{c}_1, \ldots, \bar{c}_s$ are distinct and non null, and $b_i \neq 0$ for all i, then

$$\bar{D}(s), B(s+\bar{q}), \bar{B}(s+\bar{p}) \Rightarrow \bar{C}(\bar{q}).$$

Using the results of this subsection, an alternative proof of the super-convergence of Gauss-Lobatto partitioned PRK methods can be done in the following way: The coefficients a_{ij}, $\bar{a}_{ij}$, b_i, and $\bar{b}_i$ can be determined from $C(s)$, $\bar{C}(s)$, $B(s)$, and $\bar{B}(s+1)$. The orthogonality properties related to the Gauss and Lobatto nodes c_i and $\bar{c}_i$ imply that $B(2s)$ and $\bar{B}(2s)$ (and $\bar{C}(s+1)$) are fulfilled. Then, Lemma IV.5.4 of [11] implies that $D(s)$ is satisfied, while Lemma 6 implies $\bar{D}(s)$. Finally, Theorem 8 implies that $y_1 - y(t_0+h) = O(h^{2s+1})$.

6.4 Implicit PRK methods of type 2

The most interesting implicit PRK methods of type 2 seem to be the non-partitioned PRK methods known as Lobatto IIIA, studied in detail in [12]. We will extend the ideas of the previous subsections to obtain with a different approach a generalization of the results of [12]. Moreover, the techniques developed here will be very useful in next subsection.

Let us consider a PRK method (6) of type 2. According to Theorem 2, in order to guarantee order of convergence p for the y component, in addition to (22) with $m \geq p/2$, (18) must be satisfied with $k = p - m$.

We assume that the coefficients $\bar{b}_i$ are defined by $\bar{D}(1)$. Here, we will consider PRK methods of type 2 that satisfy

$$\sum b_i(1-c_i)w_{i1} = \bar{b}_1 = 0. \tag{44}$$

This implies that $I\bar{D}(\bar{r})$ and $\bar{D}(\bar{r})$ are equivalent, as $\bar{a}_{ij}$ can be replaced by $\tilde{a}_{ij}$ in $\bar{D}(\bar{r})$.

Note that (44) is equivalent, taking into account that $\sum b_i w_{ij} = 0$, to the condition (37) for $w = ([\bullet]_1, \emptyset)$, that is

$$\sum_{i=1}^{s} b_i c_i w_{i1} = 0.$$

Under these conditions, an analog of Theorem 8 for PRK methods of type 2 can be similarly proven:

Theorem 9 *Given a PRK method (6) of type 2 such that (7) is satisfied, if there exist $\bar{b}_1 = 0, \bar{b}_2, \ldots, \bar{b}_s$ such that, the $C(q)$, $\bar{C}(\bar{q})$, $D(r)$, $\bar{D}(\bar{r})$, $B(p)$, and $\bar{B}(\bar{p})$ are fulfilled, then, the local error for the y-component of the PRK method satisfies $y_1 - y(t_0+h) = O(h^{R+1})$, where R is given by (43).*

Typically, as in the case of Lobatto IIIA methods, $c_s = 1$, and the numerical approximation for the z component is taken as $z_1 = Z_s$. Thus, under the conditions of the previous theorem, (22) is fulfilled with $p = R$, $m = \bar{q}$. But what can be said about condition (18)? Fortunately, the simplifying assumptions work for the conditions (37) of Subsection 5.4 in a similar way that for the order conditions of Subsection 5.3.

In particular, $C(q)$ and $\bar{C}(\bar{q})$ imply that conditions (37) corresponding to m-tuples $w = (u_1, \ldots, u_m, \emptyset) \in \mathcal{DT}_1^*$ with some u_l with some subtree u satisfying one of the three conditions of Lemma 5 are redundant. $D(r)$ implies that m-tuples of the form $(u_1, \ldots, u_m, \emptyset) \in \mathcal{T}_1^*$ with $u_1 = [\bullet^l]_1$, $l < r$, and $u_2 \in \mathcal{T}_1$ need not to be considered. As for $\bar{D}(\bar{r})$, it implies that condition (37) for $w = ([\bullet^l]_1, \emptyset)$ is satisfied if $l \leq \bar{r}$, and that conditions for m-tuples of the form $w = (u_1, \ldots, u_m, \emptyset) \in \mathcal{DT}_1^*$ with $u_1 = [\bullet^{l_1}]_1$, $u_2 = [\bullet^{l_2}]_2$ and $l_1 + l_2 - 1 < \bar{r}$ become redundant.

The following result can be proven using similar arguments to those of the proof of Theorem 8:

Lemma 7 *Under the hypothesis of Theorem 9, condition (18) is fulfilled with*

$$k = \min(q + 1, \bar{q}, r + 1, \bar{r} + 1).$$

Finally, Theorem 2, Theorem 9 and Lemma 7 imply the main result of this subsection:

Theorem 10 *Under the assumptions of Theorem 9, and with $c_s = 1$, $z_1 = Z_s$, and $|\alpha| \leq 1$, then, the global error of the application of the PRK method (6) with consistent initial values, for the y-component is $O(h^R)$, where R is given by (43) if $|\alpha| < 1$ and*

$$R = \min(p, \bar{p}, 2q + 1, 2\bar{q} - 1, r + q + 1, r + \bar{q} + 1, \bar{r} + q + 2, \bar{r} + \bar{q} + 1) \text{ if } |\alpha| = 1.$$

As for the global error for the z-component, it is of order $min(p, \bar{p}, q + 1, \bar{q})$ if $|\alpha| < 1$, and order $min(p, \bar{p}, q, \bar{q} - 1)$ if $|\alpha| = 1$.

Note that in the particular case of a non-partitioned Runge-Kutta method of type 2, where $\bar{p} = p, \bar{q} = q, \bar{r} = r$, the main result of [12] is recovered.

6.5 Partitioned half-explicit Runge-Kutta methods

Half-explicit methods are for DAE systems, the counterpart of explicit methods for ODEs: They are efficient, robust, and easy to implement.

A PRK method (6) to solve the system is said *half-explicit* if the matrix A is strictly lower triangular and $\bar{A}$ is lower triangular.

Half-explicit Runge-Kutta methods [9, 2, 3, 4] are particular cases of such half-explicit PRK methods (6), where (9) is satisfied, and $\bar{a}_{ii} \neq 0$ for $i = 1, \ldots, s$, so that $\bar{A}^{-1}$ is invertible, and therefore they are PRK methods of type 1.

In [13] we propose a family of half-explicit PRK methods of type 2 that satisfy $b_i = \bar{a}_{s-1,i} = a_{si}$, $d_i = 0$ for $i = 1, \ldots, s-1$, and $b_s = a_{ss} = 0$, $d_s = 1$, so that $y_1 = Y_s = \bar{Y}_s$ and $z_1 = Z_s$. In order that the method be of type 2, it is assumed that $\bar{a}_{ii} \neq 0$ for $i \geq 2$. As in [13] we will refer to this methods simply as *partitioned half-explicit Runge-Kutta (PHERK)* methods. Thus, a step $(y_0, z_0) \to (y_1, z_1)$ of a s-stage PHERK method is defined by

$$
\begin{aligned}
Y_1 &= y_0, \quad Z_1 = z_0, \\
i &= 2, \ldots, s, \\
& \qquad Y_i = y_0 + h \sum_{j=1}^{i-1} a_{ij} f(Y_j, Z_j), \\
& \qquad \overline{Y}_i = y_0 + h \sum_{j=1}^{i} \bar{a}_{ij} f(Y_j, Z_j), \quad g(\overline{Y}_i) = 0, \\
y_1 &= \bar{Y}_{s-1}, \quad z_1 = Z_s,
\end{aligned}
\tag{45}
$$

where $a_{si} = \bar{a}_{s-1,i}$ for all i ($a_{ss} = 0$) and $\bar{a}_{ii} \neq 0$ for $i \geq 2$.

Thus, the numerical approximation $y_1 \approx y(t_0 + h)$ satisfies the algebraic constraint of (1). The choice $Y_s = \bar{Y}_{s-1} = y_1$ and $z_1 = Z_s$ simplifies the order conditions for the algebraic component, and in addition, assures the equivalence, in the case of linear g, with the application of the underlying $(s-1)$-stage explicit Runge-Kutta method (with $b_i = a_{si} = \bar{a}_{s-1,i}$) to index 1 formulation (5).

Although the PHERK method (45) is formally an s-stage partitioned Runge-Kutta method (6) of type 2, its effective number of stages is $s-1$ (the same as its underlying explicit Runge-Kutta method), as $s-1$ equations have to be solved and $s-1$ new $f(Y_i, Z_i)$ are computed at each step ($f(Y_1, Z_1) = f(y_0, z_0)$ is already computed at the previous step).

Arnold [1] considered and developed, independently and approximately at the same time of [13], a new class of half-explicit methods to solve (1) that are very related to PHERK methods. In fact, these methods are precisely the interesting particular case of partitioned half-explicit Runge-Kutta methods (45) such that

$$
\bar{a}_{ij} = a_{i+1,j}, \quad 2 \leq i \leq s, \quad 1 \leq j \leq s,
$$

so that $\overline{Y}_i = Y_{i+1}$ for $2 \leq i \leq s-1$.

Methods of order up to 4 According to Theorem 2, a PHERK method (45) is of order 3 for both y and z if $|\alpha| = |w_{s1}| < 1$ and (22) are satisfied for $p = m = 3$, that is, the algebraic conditions of Table 3 are fulfilled. As the PHERK methods satisfy (7), (18) holds at least for $k = 1$, and therefore, if only convergence of order 2 is required for the algebraic variables, according to Theorem 2, the last two conditions of Table 3 need not to be satisfied.

Note that the first four equations in Table 3 only depend on A and b, and are the conditions for the corresponding explicit Runge-Kutta method to be of order 3 for ODEs. As for the rest of the conditions, according to Lemma 5, they are greatly simplified if $\bar{C}(2)$ is assumed, so that only the 9th condition remains. Thus, we have the following result:

Theorem 11 *Let us consider a s-stage PHERK method (45) such that the underlying $(s-1)$-stage explicit Runge-Kutta method is of order 3 for ODEs. If its coefficients satisfy $\bar{C}(2)$, and $|w_{s1}| < 1$, then (22) holds with $p = 3$ and $m = 1$. If in addition*

$$\sum_{i=1}^{s} w_{si}\bar{c}_i^3 = 3,$$

then (22) is fulfilled with $m = 2$.

It is then straightforward to see that, given a 3-stage explicit Runge-Kutta method of order 3 for ODEs, a 4-stage PHERK method of order 3 (for both y and z) can be constructed for each $w_{s1} \in (-1, 1)$ and $\bar{c}_2, \bar{c}_4$ (if $0, \bar{c}_2, 1, \bar{c}_4$ are distinct).

It is well known that the construction of explicit Runge-Kutta methods of order higher than 3 is best accomplished if the standard simplifying assumption $D(1)$ is made. Let us now consider s-stage PHERK methods such that $\bar{C}(2)$ and $D(1)$ are satisfied, and the underlying explicit method is of order 4: From Lemma 5 and the proof of Theorem 8 one obtains that, with assumptions $D(1)$ and $\bar{C}(2)$, the independent conditions of the form (33) and (34) for a PHERK method (45) to be of order 4 for both the differential and algebraic components are only those corresponding to explicit Runge-Kutta method of order 4, and the order conditions of the trees u, v_1, v_2, v_3, v_4 of Figure 3. However, if the order of convergence 4 is only required for the y-components, the conditions for the trees v_2, v_3, v_4 need not to be satisfied. If in addition the simplifying assumption $\bar{C}(3)$ is made, according to Lemma 5, the order conditions corresponding to the trees u, v_1, v_4 of Figure 3 become redundant. Thus, we have the following result:

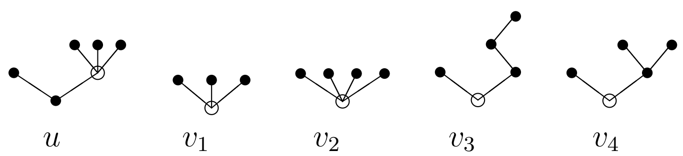


Figure 3: Additional conditions for order 4

Theorem 12 *Given a s-stage PHERK method (45) such that $D(1)$ is satisfied and the underlying explicit Runge-Kutta method is of order 4 for ODEs, if $\bar{C}(3)$ is satisfied, then*

Table 6: PHERK method of order 4

c_i	a_{ij}			
0				
$\frac{1}{3}$	$\frac{1}{3}$			
$\frac{2}{3}$	$-\frac{1}{3}$	1		
1	1	-1	1	
1	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$

$\bar{c}_i$	$\bar{a}_{ij}$				
0					
$\frac{1}{2}$	$\frac{1}{8}$	$\frac{3}{8}$			
$\frac{7}{8}$	$\frac{161}{1024}$	$\frac{147}{512}$	$\frac{441}{1024}$		
1	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$	
$\frac{9}{10}$	$\frac{693}{5000}$	$\frac{1701}{5000}$	$\frac{243}{625}$	$\frac{81}{1250}$	$-\frac{81}{2500}$

(22) holds with $p = 4$ and $m = 2$. If in addition, condition

$$\sum_i w_{si}\bar{c}_i^4 = 4, \quad \sum_{i,j,l} w_{si}\bar{c}_i\bar{a}_{ij}a_{jl}c_l = \frac{2}{3} \tag{46}$$

holds, then (22) is fulfilled with $p = 4$ and $m = 3$.

Using this result, in 45, we have presented a 5-stage PHERK method (4 effective stages) of order 4 (for both y and z) based on the classical 3/8-rule, determining the remaining parameters so that $\bar{C}(3)$ and (46) hold, and choosing the free parameters ($w_{s1} \neq 0$ and $\bar{c}_3$) in such a way that the local error coefficients and $|w_{s1}|$ are reasonably small. Its coefficients are displayed in Table 6.

Methods of order 5 and 6 The construction of higher order explicit Runge-Kutta methods for ODEs usually relies on the simplifying assumption $B(1)$ and

$$C^*(q): \quad b_2 = 0, \quad \sum_{j=1}^{i} a_{ij}c_j^{l-1} = \frac{c_i^l}{l}, \quad 3 \le i \le s, \quad 1 \le l \le q.$$

Given a s-stage PHERK method satisfying $D(1)$, $C^*(2)$, and $\bar{C}(3)$, taking into account Lemma 5 and the proof of Theorem 8, it can be seen that the only trees of T_2 of order ≤ 3 that are not simplified with these assumptions are the trees v_2 and v_3 of Figure 3. As for the trees of $\bar{T}_1$ of order ≤ 5 with some vertex of type 2, only $u_2 = [\bullet, v_2]_1$, and $u_3 = [\bullet, v_3]_1$, need to be considered.

When constructing PHERK methods of higher order, it seems interesting to consider methods satisfying (18) for $k \le 2$, so that the influence of the error for the z components on the global error for the y-components is reduced, and high order can be achieved for the differential variables with more modest order of convergence for the algebraic variables. We are now interested in PHERK methods such that (18) is satisfied for $k = 2$, that is, (39) is fulfilled. Assumption $D(1)$ and $\bar{C}(2)$ have the effect of making redundant respectively the second and third equations of (39). Let us now consider the real numbers $\bar{b}_1, \bar{b}_2, \ldots, \bar{b}_{s-2}, \bar{b}_{s-1}$ defined by $\bar{D}(1)$ (Subsection 6.3). As we have already shown in Subsection 6.4, the second equation of (18) is then equivalent to (44), so that (18) holds for $k = 2$ if (44) is fulfilled.

Assumption $\bar{D}(1)$ and (44) make the order condition for the tree $u_2 = [\bullet, v_2]_1$ equivalent to the equality of $\bar{B}(5)$ corresponding to $l = 5$, while the condition of the tree $u_3 = [\bullet, v_3]_1$ becomes equivalent to the equation (47) below. Summing up, the following result is obtained:

Theorem 13 *Let us consider a s-stage PHERK method (45) such that the underlying (s-1)-stage explicit Runge-Kutta method satisfies $D(1)$ and $C^*(2)$ and it is of order 5 for ODEs. If $\bar{C}(3)$, $\bar{D}(1)$, and $\bar{B}(5)$ are fulfilled for real numbers $\bar{b}_1, \bar{b}_2, \ldots, \bar{b}_{s-2}, \bar{b}_{s-1}$, $b_1 = 0$, and*

$$\sum_{i=2}^{s-1} \bar{b}_i \bar{c}_i \bar{a}_{i2} = 0, \tag{47}$$

holds, then (22) and (18) are satisfied with $p = 5$, $m = 3$, $k = 2$, so that, if $|w_{s1}| < 1$, the method is of order 5 for the differential variables and of order 3 for the algebraic variables. If in addition (46) is satisfied, the method is of order 4 for the algebraic variables, and the local error for the z-component does not affect the leading term of the global error for the y-component.

Taking into account $C^*(2)$, $\bar{C}(3)$ and the definition of the coefficients w_{ij}, it is straightforward to check that (46) is equivalent to the following condition: There exist $f_1 = 0, f_2, \ldots, f_{s-1}, f_s = 0$ and $g_1 = 0, g_2, \ldots, g_{s-1}, g_s = 0$ such that

$$\sum_{j=1}^{s} \bar{a}_{ij}(f_j + c_j^3) = \bar{c}_i^4, \quad \sum_{j=1}^{s} \bar{a}_{ij} g_j = \bar{c}_i \bar{a}_{i2}, \quad 2 \le i \le s. \tag{48}$$

It is not difficult to see that some of the sufficient conditions of Theorem 13 for a PHERK method to be of order 5 for the differential component are redundant. In particular, the three conditions corresponding to $\bar{B}(4)$ need not to be considered. Alternatively, if $0, \bar{c}_3, \bar{c}_4$ are distinct, the equations of $\bar{D}(1)$ corresponding to $i = 1, 3, 4$ are implied by the rest of the conditions of the theorem.

In [13], we construct, given a 6-stage explicit Runge-Kutta method of order 5 for ODEs that satisfies $D(1)$ and $C^*(2)$, a 6-parametric family of 7-stage PHERK methods (with

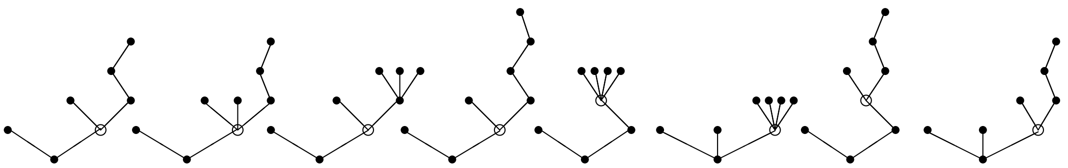


Figure 4: Remaining trees for order 6

6 effective stages) of order 5 for the differential component and order 4 for the algebraic component (satisfying (18) for $k = 2$). These methods are provided with 4th order error embedded method and dense output. A particular PHERK method whose underlying explicit Runge-Kutta method is the well known method DOPRI5 constructed by Dormand and Prince [8] (see also Section II.5 of [10]) is proposed in [13], and numerical experiments are reported.

As for the conditions for a PHERK method to be of order 6 for the differential variables, if in addition to the conditions of Theorem 13 the underlying explicit Runge-Kutta method is of order 6 for ODEs, and $C^*(3)$, $\bar{B}(6)$, and (48) are satisfied, then, the only independent order conditions of the form (33) needed for the PHERK method (45) to satisfy (22) and (18) with $p = 6$, $m = 4$, $k = 2$. are those corresponding to the trees of Figure 4. It is not difficult to see that these conditions are equivalent to the following equations:

$$\sum_{i=2}^{s-1} \bar{b}_i \bar{c}_i \bar{a}_{i2} = 0, \quad \sum_{i=2}^{s-1} \bar{b}_i \bar{c}_i^2 \bar{a}_{i2} = 0, \quad \sum_{i,j} \bar{b}_i \bar{c}_i \bar{a}_{ij} f_j = 0, \quad \sum_{i,j} \bar{b}_i \bar{c}_i \bar{a}_{ij} a_{j2} = 0,$$
$$\sum_{i,j} b_i c_i a_{ij} f_j = 0, \quad \sum_{i,j} b_i c_i^2 f_i = 0, \quad \sum_{i,j} b_i c_i a_{ij} g_j = 0, \quad \sum_{i,j} b_i c_i^2 g_i = 0.$$

References

[1] M. Arnold, *Half-Explicit Runge-Kutta Methods with Explicit Stages for Differential-Algebraic Systems of Index 2*, submitted to BIT (1995).

[2] V. Brasey *Half-Explicit Methods for Semi-Explicit Differential-Algebraic Equations of Index 2*, Ph. D. Thesis, Université de Genève, Genève (1994).

[3] V. Brasey and E. Hairer, *Half-Explicit Runge-Kutta Methods for Differential-Algebraic Systems of Index 2*, Siam J. Numer. Anal., Vol. 30, No. 2, 538-552 (1993).

[4] V. Brasey, *A Half-Explicit Runge-Kutta Method of Order 5 for Solving Constrained Mechanical Systems*, Computing 48, 191-201 (1992).

[5] K. E. Brenan, S. L. Campbell, and L. R. Petzold, *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*, North-Holland, New-York, (1989).

[6] K. E. Brenan and L. R. Petzold, *The Numerical Solution of higher index Differential/Algebraic Equations by Implicit Runge-Kutta Methods*, SIAM J. Numer. Anal., 26, 976-996 (1989).

[7] J. C. Butcher, *The Numerical Analysis of Ordinary Differential Equations*, John Wiley & Sons (1987).

[8] J. R. Dormand and P. J. Prince, *A Family of Embedded Runge-Kutta Formulae*, J. Comp. Appl. Math., Vol.6, 19-26 (1980).

[9] E. Hairer, Ch. Lubich, M. Roche, *The Numerical Solution of Differential-Algebraic Systems by Runge-Kutta Methods*, Lecture-Notes in Mathematics, Vol 1409, Springer-Verlag (1989).

[10] E. Hairer, S.P. Nørset, G. Wanner: *Solving Ordinary Differential Equations I. Nonstiff Problems*, Second Edition, Springer-Verlag (1993).

[11] E. Hairer, G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*, Springer-Verlag (1991).

[12] L. Jay, *Convergence of a Class of Runge-Kutta Methods for Differential-Algebraic Systems of Index 2*, BIT, 137-150 (1993).

[13] A. Murua, *Partitioned Half-Explicit Runge-Kutta Methods for Differential-Algebraic Systems of Index 2*, Computing 59, 43–61 (1997).

[14] A. Murua, *Formal Series and Numerical Integrators, Part II: Application to Index 2 Differential-Algebraic Systems*, Appl. Num. Math. 29, 99–113 (1999).