A general family of pseudo two-step Runge-Kutta methods *

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Abstract

The aim of this paper is to design a new family of numerical methods of arbitrarily high order for systems of first-order differential equations which are to be termed pseudo two-step Runge-Kutta methods. By using collocation techniques, we can obtain an arbitrarily high-order stable pseudo two-step Runge-Kutta method with any desired number of implicit stages in retaining the two-step nature. In very first investigations, the pseudo two-step Runge-Kutta methods are shown to be promising numerical integration methods.

Key words: Runge-Kutta methods, two-step Runge-Kutta methods, zero-stability, parallelism.
AMS(MOS) subject classifications (1991): 65M12, 65M20
CR subject classifications: G.1.7

1 Introduction

We will design a new family of numerical methods for solving the initial value problem (IVP) for the system of first-order, ordinary differential equations (ODEs)

$$\mathbf{y}'(t) = \mathbf{f}(\mathbf{y}(t)), \qquad \mathbf{y}(t_0) = \mathbf{y}_0, \qquad t_0 \le t \le T, \tag{1.1}$$

where $\mathbf{y}$, $\mathbf{f} \in \mathbb{R}^d$. In the literature there have been proposed the best IRK methods with w implicit stages of stage order w and step order $2w$ (Gauss-Legendre IRK methods). The new methods considered in this paper which will be termed *pseudo two-step RK methods (PTRK methods)* are based on an approach which enables us to derive the methods of any given order of accuracy with any desired number of implicit stages. When compared with the classical IRK methods, the new family of PTRK methods has an advantage of being of order $2w$ for both step point and stage with the number implicit stages arbitrarily less than w. With $w = 1$, the PTRK methods have the same computational complexity as the implicit LM methods but they can be of arbitrarily high order in retaining the two-step nature and zero-stability. The main idea of the approach used in this paper is similar to that of the approach used in [4, 6] and the two-step nature of PTRK methods is also of the

*This work was partly supported by DAAD, N.R.P.F.S. and QG-96-02

similar concept but the definition of the PTRK methods gives much more freedom in the choice of method parameters. More precisely, the choice of collocation vectors of the methods considered in [4] is restricted by the zero-stability requirement. Whereas, PTRK methods are always zero-stable for any set of collocation abscissas. The class of explicit PTRK methods investigated in [8] as a special case of the family of PTRK methods considered in this paper while these PTRK methods have no implicit stages, is shown to be superior to the most efficient sequential and parallel methods currently available in the literature.
Similarly to the methods considered in [4, 6], the PTRK methods also fall into the class of general linear methods (GLM) (cf. e.g., [2, 11]). However, the parameters of PTRK methods are easily to be derived and the methods themself are applicable to parallel computations based on the approach used in e.g., [3, 5, 7, 12, 13].
In Section 2 we will define and investigate the PTRK methods where order conditions, zero-stability aspect and an option for the choice of the method parameters are considered. Furthermore, in Section 3, we present a numerical test showing the theoretical performance of PTRK methods.
In the following sections, for the sake of simplicity of notation, we assume that the IVP (1.1) is a scalar problem. However, all considerations below can be straightforwardly extended to a system of ODEs, and therefore, also to nonautonomous equations.

2 Pseudo two-step RK methods

Let a chosen s-dimensional collocation vector $\mathbf{c}$ be partitioned into two subvectors $\mathbf{c}_v$ and $\mathbf{c}_w$ that is $\mathbf{c} = (\mathbf{c}_v^T, \mathbf{c}_w^T)^T$, then a general s-stage PTRK method based on $\mathbf{c}$ for a scalar authonomous equation is defined by

$$\mathbf{Y}_n^v = y_n\mathbf{e}_v + hA_{vv}f(\mathbf{Y}_{n-1}^v) + hA_{vw}f(\mathbf{Y}_{n-1}^w), \tag{2.1a}$$

$$\mathbf{Y}_n^w = y_n\mathbf{e}_w + hA_{wv}f(\mathbf{Y}_n^v) + hA_{ww}f(\mathbf{Y}_n^w), \tag{2.1b}$$

$$y_{n+1} = y_n + h\mathbf{b}_v^T f(\mathbf{Y}_n^v) + h\mathbf{b}_w^T f(\mathbf{Y}_n^w), \tag{2.1c}$$

where, $y_{n+1} \approx y(t_{n+1})$, h is the stepsize, A_{ij} are $i\times j$ method parameter matrices, $\mathbf{b}_j$ and $\mathbf{c}_j$ are j-dimensional method parameters vectors, $\mathbf{e}_j$ is the j-dimensional vectors with unit entries, (for $i, j = v, w; v+w = s$). $\mathbf{Y}_n^v$ is the so called explicit stage subvector representing the numerical approximation to the exact solution vector $y(t_n\mathbf{e}_v + \mathbf{c}_v h) = [y(t_n + c_1 h), \ldots, y(t_n + c_v h)]^T$ and $\mathbf{Y}_n^w$ denotes the so called implicit stage subvector representing numerical approximation to the exact solution vector $y(t_n\mathbf{e}_w + \mathbf{c}_w h) = [y(t_n + c_{v+1}h), \ldots, y(t_n + c_s h)]^T$ at nth step, respectively. The method parameters matrices and vectors A_{ij}, $\mathbf{b}_j$ will be determined by order conditions (see Section 2.1). Furthermore, in (2.1) and elsewhere in this paper, we use for any vector $\mathbf{v} = (v_1, \ldots, v_s)^T$ and any scalar function $f(t)$ the notation $f(\mathbf{v}) := [f(v_1), \ldots, f(v_s)]^T$. For presentational convenience, we specify this PTRK method by the tableau

$$\begin{array}{cc|c|cc} A_{vv} & A_{vw} & \mathbf{c}_v & O_{vv} & O_{vw} \\ O_{wv} & O_{ww} & \mathbf{c}_w & A_{wv} & A_{ww} \\ \hline & & y_{n+1} & \mathbf{b}_v^T & \mathbf{b}_w^T \end{array} \tag{2.2}$$

In order to start the method (2.1), an appropriate starting procedure is needed for generating sufficiently accurate starting vector $\mathbf{Y}_0 = [(\mathbf{Y}_0^v)^T, (\mathbf{Y}_0^w)^T]^T$ from y_0. This can be done, for example, by using an appripriate RK-type method.
The s-stage PTRK method (2.1) consists of v explicit stages and w implicit stages. The order of PTRK method (2.1) can be studied in the same way as the order of RK methods. Thus suppose that $y_n = y(t_n)$ and $\mathbf{Y}_{n-1} = y(t_{n-1}\mathbf{e} + h\mathbf{c})$. Then we have the following order definition

Definition 2.1 *The PTRK method (1.1) is said to be of order* p^* *if*

$$y(t_{n+1}) - y_{n+1} = O(h^{p^*+1}),$$

and stage order $q^* = min\{p^*, q_1, q_2\}$ *if in addition,*

$$\begin{aligned} y(t_n\mathbf{e}_v + h\mathbf{c}_v) - \mathbf{Y}_n^v &= O(h^{q_1+1}), \\ y(t_n\mathbf{e}_w + h\mathbf{c}_w) - \mathbf{Y}_n^w &= O(h^{q_2+1}). \end{aligned}$$

Notice that the local stage order equals $q_1 + 1$ for the explicit stages and equals $q_2 + 1$ for the implicit stages. In the next section we will consider the order conditions for the PTRK methods.

2.1 Order conditions

In this section we consider order conditions for the PTRK methods. For the (fixed) stepsize h, the respective orders q_1, q_2 and p conditions for (2.1a), (2.1b) and (2.1c) are derived by replacing $\mathbf{Y}_{n-1}^v$, $\mathbf{Y}_{n-1}^w$, y_n, $\mathbf{Y}_n^v$, $\mathbf{Y}_n^w$ and y_{n+1} by the exact solution values $y(t_{n-1}\mathbf{e}_v + h\mathbf{c}_v) = y(t_n\mathbf{e}_v + h(\mathbf{c}_v - \mathbf{e}_v))$, $y(t_{n-1}\mathbf{e}_w + h\mathbf{c}_w) = y(t_n\mathbf{e}_w + h(\mathbf{c}_w - \mathbf{e}_w))$, $y(t_n)$, $y(t_n\mathbf{e}_v + h\mathbf{c}_v)$, $y(t_n\mathbf{e}_w + h\mathbf{c}_w)$ and $y(t_{n+1}) = y(t_n + h)$, respectively. On substitution of these exact solution values into (2.1), we are led to

$$\begin{aligned} y(t_n\mathbf{e}_v + h\mathbf{c}_v) - y(t_n\mathbf{e}_v) - hA_{vv}y'(t_n\mathbf{e}_v + h(\mathbf{c}_v - \mathbf{e}_v)) \\ - hA_{vw}y'(t_n\mathbf{e}_w + h(\mathbf{c}_w - \mathbf{e}_w)) = O(h^{q_1+1}), \end{aligned} \tag{2.3a}$$

$$\begin{aligned} y(t_n\mathbf{e}_w + h\mathbf{c}_w) - y(t_n\mathbf{e}_w) - hA_{wv}y'(t_n\mathbf{e}_v + h\mathbf{c}_v) \\ - hA_{ww}y'(t_n\mathbf{e}_w + h\mathbf{c}_w) = O(h^{q_2+1}), \end{aligned} \tag{2.3b}$$

$$\begin{aligned} y(t_n + h) - y(t_n) - h\mathbf{b}_v^T y'(t_n\mathbf{e}_v + h\mathbf{c}_v) \\ - h\mathbf{b}_w^T y'(t_n\mathbf{e}_w + h\mathbf{c}_w) = O(h^{p+1}). \end{aligned} \tag{2.3c}$$

Using Taylor expansions for the sufficiently smooth function y(t) in the neighbourhood of t_n, we can expand the left-hand sides of (2.3) in powers of h and obtain

$$\begin{aligned} &\left[exp\left(h\mathbf{c}_v\frac{d}{dt}\right) - y(t_n\mathbf{e}_v) - hA_{vv}\frac{d}{dt}exp\left(h(\mathbf{c}_v - \mathbf{e}_v)\frac{d}{dt}\right) - hA_{vw}\frac{d}{dt}exp\left(h(\mathbf{c}_w - \mathbf{e}_w)\frac{d}{dt}\right)\right]y(t_n) \\ &= \sum_{j=1}^{q_1}\mathbf{C}_v^{(j)}\left(h\frac{d}{dt}\right)^j y(t_n) + \mathbf{C}_v^{(q_1+1)}\left(h\frac{d}{dt}\right)^{q_1+1} y(t_v^*) = O(h^{q_1+1}), \end{aligned} \tag{2.4a}$$

$$\left[exp\left(h\mathbf{c}_w\frac{d}{dt}\right)-y(t_n\mathbf{e}_w)-hA_{wv}\frac{d}{dt}exp\left(h\mathbf{c}_v\frac{d}{dt}\right)-hA_{ww}\frac{d}{dt}exp\left(h\mathbf{c}_w\frac{d}{dt}\right)\right]y(t_n)$$
$$=\sum_{j=1}^{q_2}\mathbf{C}_w^{(j)}\left(h\frac{d}{dt}\right)^j y(t_n)+\mathbf{C}_w^{(q_2+1)}\left(h\frac{d}{dt}\right)^{q_2+1}y(t_w^*)=O(h^{q_2+1}), \tag{2.4b}$$

$$\left[exp\left(h\frac{d}{dt}\right)-y(t_n)-h\mathbf{b}_v^T\frac{d}{dt}exp\left(h\mathbf{c}_v\frac{d}{dt}\right)-h\mathbf{b}_w^T\frac{d}{dt}exp\left(h\mathbf{c}_w\frac{d}{dt}\right)\right]y(t_n)$$
$$=\sum_{j=1}^{p}D^{(j)}\left(h\frac{d}{dt}\right)^j y(t_n)+D^{(p+1)}\left(h\frac{d}{dt}\right)^{p+1}y(t^*)=O(h^{p+1}), \tag{2.4c}$$

where, t_v^*, t_w^* and t^* are suitably chosen points in the interval $[t_{n-1},t_{n+1}]$, and

$$\mathbf{C}_v^{(j)}=\frac{1}{j!}\big[\mathbf{c}_v^j-jA_{vv}(\mathbf{c}_v-\mathbf{e}_v)^{j-1}-jA_{vw}(\mathbf{c}_w-\mathbf{e}_w)^{j-1}\big], \qquad j=1,\dots,q_1, \tag{2.5a}$$
$$\mathbf{C}_w^{(j)}=\frac{1}{j!}\big[\mathbf{c}_w^j-jA_{wv}\mathbf{c}_v^{j-1}-jA_{ww}\mathbf{c}_w^{j-1}\big], \qquad j=1,\dots,q_2, \tag{2.5b}$$
$$D^{(j)}=\frac{1}{j!}\big[1-j\mathbf{b}_v^T\mathbf{c}_v^{j-1}-j\mathbf{b}_w^T\mathbf{c}_w^{j-1}\big], \qquad j=1,\dots,p. \tag{2.5c}$$

The vectors $\mathbf{C}_v^{(j)}$, $\mathbf{C}_w^{(j)}$ and the scalars $D^{(j)}$ represent the error vectors of the stage numerical approximations (2.1a), (2.1b) and the error terms of the step numerical approximation (2.1c), respectively. From (2.4), we obtain the order conditions

$$\mathbf{C}_v^{(j)}=\mathbf{0}, \qquad j=1,\dots,q_1, \tag{2.5d}$$
$$\mathbf{C}_w^{(j)}=\mathbf{0}, \qquad j=1,\dots,q_2, \tag{2.5e}$$
$$D^{(j)}=0, \qquad j=1,\dots,p. \tag{2.5f}$$

The vectors $\mathbf{C}_v^{(q_1+1)}$, $\mathbf{C}_w^{(q_2+1)}$, and the scalar $D^{(p+1)}$ are the *principal* error vectors and error term of the numerical approximations in (2.1). The conditions (2.5), imply that the local step and stage orders satisfy the order relations

$$\begin{aligned} y(t_n\mathbf{e}_v+h\mathbf{c}_v)-\mathbf{Y}_n^v&=O(h^{q_1+1}),\\ y(t_n\mathbf{e}_w+h\mathbf{c}_w)-\mathbf{Y}_n^w&=O(h^{q_2+1}),\\ y(t_{n+1})-y(t_n)-h\mathbf{b}_v^Tf(y(t_n\mathbf{e}_v+h\mathbf{c}_v))&\\ -h\mathbf{b}_w^Tf(y(t_n\mathbf{e}_w+h\mathbf{c}_w))&=O(h^{p+1}). \end{aligned} \tag{2.6}$$

Theorem 2.1 *If the function f is Lipschitz continous, and if*

$$(A_{vv},A_{vw})(\mathbf{c}-\mathbf{e})^{j-1}=\frac{\mathbf{c}_v^j}{j}, \qquad j=1,\dots,q_1, \tag{2.7a}$$
$$(A_{wv},A_{ww})\mathbf{c}^{j-1}=\frac{\mathbf{c}_w^j}{j}, \qquad j=1,\dots,q_2, \tag{2.7b}$$
$$(\mathbf{b}_v^T,\mathbf{b}_w^T)\mathbf{c}^{j-1}=\frac{1}{j}, \qquad j=1,\dots,p, \tag{2.7c}$$

then the PTRK method (2.1) has order $p^* = min\{p, q_1 + 1, q_2 + 1\}$ *and stage order* $q^* = min\{p, q_1, q_2\}$ *for any collocation vector* $\mathbf{c}$ *with distinct abscissas* c_i *and for any integers* v *and* w, $w + v = s$.

Proof. Suppose that $y_n = y(t_n)$, $\mathbf{Y}^v_{n-1} = y(t_{n-1}\mathbf{e}_v + h\mathbf{c}_v)$ and $\mathbf{Y}^w_{n-1} = y(t_{n-1}\mathbf{e}_w + h\mathbf{c}_w)$. Since conditions (2.5) and (2.7) are equivalent, and f is Lipschitz continous, from (2.6), we obtain the following order relation

$$\begin{aligned} y(t_{n+1}) - y_{n+1} &= y(t_{n+1}) - y(t_n) - h\mathbf{b}_v^T f(y(t_n\mathbf{e}_v + h\mathbf{c}_v)) - h\mathbf{b}_w^T f(y(t_n\mathbf{e}_w + h\mathbf{c}_w)) \\ &\quad + h\mathbf{b}_v^T[f(y(t_n\mathbf{e}_v + h\mathbf{c}_v)) - f(\mathbf{Y}^v_n)] + h\mathbf{b}_w^T[f(y(t_n\mathbf{e}_w + h\mathbf{c}_w)) - f(\mathbf{Y}^w_n)] \\ &= O(h^{p+1}) + O(h)[y(t_n\mathbf{e}_v + h\mathbf{c}_v) - \mathbf{Y}^v_n] + O(h)[y(t_n\mathbf{e}_w + h\mathbf{c}_w) - \mathbf{Y}^w_n] \\ &= O(h^{p+1}) + O(h^{q_1+2}) + O(h^{q_2+2}) \end{aligned} \tag{2.8}$$

by which Theorem 2.1 is proved. ■

In order to express the parameter matrices A_{vv}, A_{vw}, A_{wv}, A_{ww} and vectors $\mathbf{b}_v$, $\mathbf{b}_w$ explicitly in terms of the collocation vector $\mathbf{c}$, we define the matrices and vector

$$P_v := \Big(\mathbf{c}_v, \frac{\mathbf{c}_v^2}{2}, \frac{\mathbf{c}_v^3}{3}, \frac{\mathbf{c}_v^4}{4} \ldots, \frac{\mathbf{c}_v^s}{s}\Big), \qquad P_w := \Big(\mathbf{c}_w, \frac{\mathbf{c}_w^2}{2}, \frac{\mathbf{c}_w^3}{3}, \frac{\mathbf{c}_w^4}{4} \ldots, \frac{\mathbf{c}_w^s}{s}\Big),$$

$$\mathbf{g} := \Big(1, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}, \ldots, \frac{1}{s}\Big)^T, \qquad R := \Big(\mathbf{e}, \mathbf{c}, \mathbf{c}^2, \mathbf{c}^3, \mathbf{c}^4, \ldots, \mathbf{c}^{s-1}\Big),$$

$$Q := \Big(\mathbf{e}, (\mathbf{c} - \mathbf{e}), (\mathbf{c} - \mathbf{e})^2, (\mathbf{c} - \mathbf{e})^3, \ldots, (\mathbf{c} - \mathbf{e})^{s-1}\Big).$$

Then the order conditions (2.5) can be presented in the form

$$(A_{vv}, A_{vw})Q - P_v = O, \quad (A_{wv}, A_{ww})R - P_w = O, \quad (\mathbf{b}_v^T, \mathbf{b}_w^T)R - \mathbf{g}^T = 0. \tag{2.9}$$

Since the components c_i of the vector $\mathbf{c}$ are assumed to be distinct implying that Q and R are nonsingular, and from (2.9), we may write

$$(A_{vv}, A_{vw}) = P_v Q^{-1}, \quad (A_{wv}, A_{ww}) = P_w R^{-1}, \quad (\mathbf{b}_v^T, \mathbf{b}_w^T) = \mathbf{g}^T R^{-1}. \tag{2.10}$$

Notice that condition (2.7c) (equivalent to (2.5f)) defines the coefficients (c_i, b_i) of a quadrature formula of order p (they satisfy the simplifying assumption $B(p)$) so that p at least equals s. With a special choice of the vector $\mathbf{c}$, it is possible to increase the order p beyond s (superconvergence) by satisfying the orthogonality relation (see [11, p. 207]). We have the following theorem which is similar to the one formulated in [8], as a simple consequence of Theorem 2.1, the explicit expressions of parameters of the PTRK methods and the application of the orthogonality relation.

Theorem 2.2 *An* s*-stage PTRK method defined by (2.1) is of step order* $p^* = s$ *and of stage order* $q^* = s$ *if the parameter matrices* A_{vv}, A_{vw}, A_{wv}, A_{ww} *and vectors* $\mathbf{b}_v$, $\mathbf{b}_w$ *of the method satisfy the relations (2.10) for any collocation vector* $\mathbf{c}$ *with distinct abscissas* c_i *and for any integers* v *and* w *with* $w + v = s$. *It has order* $p^* = s + 1$ *if in addition*

$$P_j(1) = 0, \qquad P_j(x) := \int_0^x \xi^{j-1} \prod_{i=1}^{s} (\xi - c_i) d\xi, \qquad j \geq 1.$$

Theorem 2.2 indicates that for an s-stage PTRK method, the maximal attainable order is $s+1$. According to the analysis of the local errors in this section, the starting values $\mathbf{Y}_0$ should be of order $s+1$ that is

$$y(t_0\mathbf{e}+h\mathbf{c})-\mathbf{Y}_0=O(h^{s+1}).$$

Remark 2.1 The PTRK methods (2.1) can also be defined via the associated IRK methods following the approaches used in [4, 6]. However, the direct formulation above gives a more detailed specification of the method parameters.

Remark 2.1 In the definition of the PTRK methods if we use the convention that a metrix having no row or no column will be the empty matrix i.e., an $i\times j$ matrix $M_{ij}=\varnothing$ iff $i=0$ or $j=0$, then a PTRK method becomes an IRK method if $v=0$ ($w=s$) and reduces to an explicit PTRK method studied in [8] if $w=0$ ($v=s$) (see Table 2.1). For an illustration

$$\begin{array}{c|c|c} O & \mathbf{c} & A \\ \hline & y_{n+1} & \mathbf{b}^T \end{array} \iff \begin{array}{cc|c|cc} A_{vv} & A_{vw} & \mathbf{c}_v & O_{vv} & O_{vw} \\ O_{wv} & O_{ww} & \mathbf{c}_w & A_{wv} & A_{ww} \\ \hline & & y_{n+1} & \mathbf{b}_v^T & \mathbf{b}_w^T \end{array} \iff \begin{array}{c|c|c} \widetilde{A} & \mathbf{c} & O \\ \hline & y_{n+1} & \mathbf{b}^T \end{array}$$

Table 2.1: Relationship between IRK, PTRK and EPTRK methods

of this relationship, we give the following examples:

Example 2.1 For the first example we consider various third-order methods based on the two-dimensional Radau IIA collocation vector $\mathbf{c}=(\frac{1}{3},1)^T$. Using explicit expressions of the parameter matices and vectors defined by (2.10), we determined the parameters of various methods as in following tableaux (see Table 2.1) and Theorem 2.2).

$$\begin{array}{cc|c|cc} 0 & 0 & \frac{1}{3} & \frac{5}{12} & -\frac{1}{12} \\ 0 & 0 & 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & & y_{n+1} & \frac{3}{4} & \frac{1}{4} \end{array} \tag{2.11a}$$

$$\begin{array}{cc|c|cc} -\frac{1}{12} & \frac{5}{12} & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 1 & \frac{3}{4} & \frac{1}{4} \\ \hline & & y_{n+1} & \frac{3}{4} & \frac{1}{4} \end{array} \tag{2.11b}$$

$$\begin{array}{cc|c|cc} -\frac{1}{12} & \frac{5}{12} & \frac{1}{3} & 0 & 0 \\ -\frac{3}{4} & \frac{7}{4} & 1 & 0 & 0 \\ \hline & & y_{n+1} & \frac{3}{4} & \frac{1}{4} \end{array} \tag{2.11c}$$

Example 2.2 For the second example we consider various third-order methods based on the three-dimensional collocation vector $\mathbf{c} = (-\frac{1}{4}, 0, \frac{3}{4})^T$. The specifications of parameters of various methods are given by the taleaux

$$\begin{array}{ccc|c|ccc} 0 & 0 & 0 & -\frac{1}{4} & -\frac{11}{96} & -\frac{5}{36} & \frac{1}{288} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{4} & -\frac{9}{32} & \frac{3}{4} & \frac{9}{32} \\ \hline & & & y_{n+1} & -\frac{1}{6} & \frac{5}{9} & \frac{11}{8} \end{array} \tag{2.12a}$$

$$\begin{array}{ccc|c|ccc} -\frac{11}{96} & \frac{7}{36} & -\frac{95}{288} & -\frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{4} & -\frac{9}{32} & \frac{3}{4} & \frac{9}{32} \\ \hline & & & y_{n+1} & -\frac{1}{6} & \frac{5}{9} & \frac{11}{8} \end{array} \tag{2.12b}$$

$$\begin{array}{ccc|c|ccc} -\frac{11}{96} & \frac{7}{36} & -\frac{95}{144} & -\frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{87}{32} & -\frac{17}{4} & \frac{73}{32} & \frac{3}{4} & 0 & 0 & 0 \\ \hline & & & y_{n+1} & -\frac{1}{6} & \frac{5}{9} & \frac{11}{8} \end{array} \tag{2.12c}$$

Example 2.3 The third example is various fourth-order methods based on the three-dimensional Lobatto collocation vector $\mathbf{c} = (0, \frac{1}{2}, 1)^T$. The parameters of various methods are defined by

$$\begin{array}{ccc|c|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 0 & 0 & 0 & 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & & & y_{n+1} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \tag{2.13a}$$

$$\begin{array}{ccc|c|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{5}{24} & -\frac{2}{3} & \frac{23}{24} & \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & & & y_{n+1} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array} \tag{2.13b}$$

$$
\begin{array}{ccc|c|ccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{5}{24} & -\frac{2}{3} & \frac{23}{24} & \frac{1}{2} & 0 & 0 & 0 \\
\frac{7}{6} & -\frac{10}{3} & \frac{19}{6} & 1 & 0 & 0 & 0 \\
\hline
 & & & y_{n+1} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
\tag{2.13c}
$$

Example 2.4 The fourth example is various fourth-order methods based on the four-dimensional collocation vector $\mathbf{c} = (0, \frac{1}{2}, 1, \frac{3}{2})^T$. The parameters of various methods are specified also by

$$
\begin{array}{cccc|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} & \frac{3}{16} & \frac{19}{48} & -\frac{5}{48} & \frac{1}{48} \\
0 & 0 & 0 & 0 & 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 \\
0 & 0 & 0 & 0 & \frac{3}{2} & \frac{3}{16} & \frac{9}{16} & \frac{9}{16} & \frac{3}{16} \\
\hline
 & & & & y_{n+1} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0
\end{array}
\tag{2.14a}
$$

b

$$
\begin{array}{cccc|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{48} & -\frac{5}{48} & \frac{19}{48} & \frac{3}{16} & \frac{1}{2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 \\
0 & 0 & 0 & 0 & \frac{3}{2} & \frac{3}{16} & \frac{9}{16} & \frac{9}{16} & \frac{3}{16} \\
\hline
 & & & & y_{n+1} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0
\end{array}
\tag{2.14b}
$$

$$
\begin{array}{cccc|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{48} & -\frac{5}{48} & \frac{19}{48} & \frac{3}{16} & \frac{1}{2} & 0 & 0 & 0 & 0 \\
-\frac{1}{6} & \frac{2}{3} & -\frac{5}{6} & \frac{4}{3} & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{3}{2} & \frac{3}{16} & \frac{9}{16} & \frac{9}{16} & \frac{3}{16} \\
\hline
 & & & & y_{n+1} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0
\end{array}
\tag{2.14c}
$$

$$
\begin{array}{cccc|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{48} & -\frac{5}{48} & \frac{19}{48} & \frac{9}{48} & \frac{1}{2} & 0 & 0 & 0 & 0 \\
-\frac{1}{6} & \frac{2}{3} & -\frac{5}{6} & \frac{4}{3} & 1 & 0 & 0 & 0 & 0 \\
-\frac{21}{16} & \frac{81}{16} & -\frac{111}{16} & \frac{75}{16} & \frac{3}{2} & 0 & 0 & 0 & 0 \\
\hline
 & & & & y_{n+1} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0
\end{array}
\tag{2.14d}
$$

Methods (2.11a) and (2.13a) are the Radau IIA and Lobatto IIIA IRK methods. Methods (2.12a) and (2.14a) are the third-order and fourth-order IRK methods. Methods (2.11b), (2.12b), (2.13b), (2.14b) and (2.14c) are the PTRK methods under considerations. They have one or two implicit stages with the same step and stage order as the associated IRK methods. Methods (2.11c), (2.12c), (2.13c) and (2.14d) are the explicit PTRK methods considered in [8]. These explicit PTRK methods have the same step and stage order as the associated with them implicit methods.

2.2 Zero-stability of PTRK methods

Since the PTRK method (2.1) is of the two-step nature, we have to check its property of zero-stability by applying (2.1) to the model test equation $y'(t) = \lambda y(t)$, where λ runs through the eigenvalues of the Jacobian matrix $\partial \mathbf{f}/\partial \mathbf{y}$ which are supposed to be lying in the left half-plane. Although we may derive the stability matrix of the method, it is more convenient to write the PTRK method (2.1) in the form of a general linear method (GLM) (see e.g., [2]). By defining the vectors

$$\mathbf{Z}_n = \left((\mathbf{Y}_n^v)^T, (\mathbf{Y}_n^w)^T, y_{n+1}\right)^T, \qquad \mathbf{Z}_{n-1} = \left((\mathbf{Y}_{n-1}^v)^T, (\mathbf{Y}_{n-1}^w)^T, y_n\right)^T, \tag{2.15}$$

the PTRK method (2.1) can be written in the GLM form

$$\mathbf{Z}_n = V\mathbf{Z}_{n-1} + hWf(\mathbf{Z}_n) \tag{2.16}$$

where the $(s+1)\times(s+1)$ matrices V and W are given by

$$V = \begin{pmatrix} O_{vv} & O_{vw} & \mathbf{e}_v \\ O_{wv} & O_{ww} & \mathbf{e}_w \\ \mathbf{0}_v^T & \mathbf{0}_w^T & 1 \end{pmatrix}, \qquad W = \begin{pmatrix} A_{vv} & A_{vw} & \mathbf{0}_v \\ A_{wv} & A_{ww} & \mathbf{0}_w \\ \mathbf{b}_v^T & \mathbf{b}_w^T & 0 \end{pmatrix}. \tag{2.17}$$

In (2.17) O_{ij} and $\mathbf{0}_i$ denote the $i \times j$ matrices and the i-dimensional vectors with zero entries. It is evident that V is a stable matrix (cf. [2]). Thus, we have

Theorem 2.3 *The pseudo two-step RK methods based on any colocation vectors* $\mathbf{c}$ *of the stage abscissas are always zero-stable for any integers* v *and* w *with* $v + w = s$.

A more detailed stability investigation involved with the construction of PTRK methods possessing large stability regions and also their stability plots will be considered in the forthcoming paper.

2.3 On the choice of method parameters

In the application of PTRK methods, for any given collocation vector $\mathbf{c}$, for the stage abscissas, the method parameters matrices A_{ij} and vectors $\mathbf{b}_j$, (for $i, j = v, w$) can be easily determined using the explicit expressions (2.10). In this way we can obtain PTRK methods of arbitrarily high order. The freedom in the choice of the collocation points c_i of the vector

$\mathbf{c}$ can be used for obtaining some useful method properties. It seems natural to choose the abscissas of the vector $\mathbf{c}$ such that the associated PTRK method has the highest possible order $s+1$ (cf. Therem 2.2) or good stability behaviour, etc. An other option followed by the same approach used in [8], minimizes the maximum norm $\|\mathbf{C}_v^{(s+1)}\|_\infty$ of the principal error vector defined by (2.5a) associated with the formula (2.4a) for the explicit stage subvector $\mathbf{Y}_n^v$. In this paper we confine our considerations to the latter option. Although we may use (2.5a) for minimizing this norm, it is more convenient to use the usual expression for the remainder term in Lagrange interpolation formulas. Using r-point Lagrange interpolation formula for sufficiently differentiable function $y(t)$(see e.g., [1, formulas 25.2.1-25.2.3])

$$y'(t_n + \tau h) = \sum_{i=1}^{r} l_i(\tau) y'(t_n + a_i h) + C^{(r)}(\tau)\left(h\frac{d}{dt}\right)^r y(t_\tau^*),$$

$$l_i(\tau) = \prod_{j=1, j\neq i}^{r} \frac{(\tau - a_j)}{(a_i - a_j)}, \qquad C^{(r)}(\tau) = \frac{1}{r!}\prod_{j=1}^{r}(\tau - a_j), \tag{2.18}$$

where, t_τ^* is a suitably chosen point in the interval $[t_n, t_n + \tau h]$, we have the following alternative form of (2.4a) (with $q_1 = s$)

$$\begin{aligned} y(t_n + c_k h) = y(t_n) + h\sum_{i=1}^{s} l_i(1 + c_k) y'(t_n + (c_i - 1)h) \\ + C^{(s+1)}(1 + c_k)\left(h\frac{d}{dt}\right)^{s+1} y(t_k^*), \qquad k = 1, \ldots, v, \end{aligned} \tag{2.19}$$

where, t_k^* is also a suitably chosen point in the interval $[t_{n-1}, t_{n+1}]$. The principal error vector in the formulas (2.4a) is given by $\mathbf{C}_v^{(s+1)} = C^{(s+1)}(\mathbf{e}_v + \mathbf{c}_v)$, so that we are led to minimize the magnitude of the values

$$C^{(s+1)}(1 + c_k) = \frac{1}{(s+1)!}\prod_{i=1}^{r}(1 + c_k - c_i), \qquad k = 1, \ldots, v. \tag{2.20}$$

From (2.20) we see that $C^{(s+1)}(1 + c_k)$ vanishes if the set of components of the vector $\mathbf{c}$ contains the components $c_k + 1$ (cf. e.g., [5, 6]). Thus we have the following theorem

Theorem 2.4 *If the set of components of vector* $\mathbf{c}$ *contains the set of components of vector* $\mathbf{c}_v + \mathbf{e}_v$*, then the principal error vector* $\mathbf{C}_v^{(s+1)}$ *has vanishing components (i.e.,* $\|\mathbf{C}_v^{(s+1)}\|_\infty = \mathbf{0}$*)*

In the forthcoming paper [9] we will construct PTRK methods based on the collocation vector $\mathbf{c}$ which satisfy the conditions of Theorem 2.4. We do not claim that this choice of method parameters is the best possible. A further study of this topic will be subject of future research.

3 Numerical test

We confine our test on the implicit PTRK methods. For the explicit ones we reffer to [8]. We apply the implicit PTRK methods (2.11b), (2.12b), (2.13b), (2.14b) and (2.14c) in four examples of Section 2.1 to the problem for equation of motion of a rigid body without external forces (cf. e.g., [14], [11, problem JACB, p. 236])

$$\begin{aligned} y_1'(t) &= y_2(t)y_3(t), & y_1(0) &= 0, & & \\ y_2'(t) &= -y_1(t)y_3(t), & y_2(0) &= 1, & 0 \le t \le T. & \\ y_3'(t) &= -0.51 y_1(t)y_2(t), & y_3(0) &= 1. & & \end{aligned} \tag{3.1}$$

The values of number of correct decimal digits NCD obtained at the end point of the integration interval for a given total number of integration steps N_{steps} (cf. e.g., [6]) listed in Table 3.2 nicely show the theoretical order behaviour of the (implicit) PTRK methods from our examples. We note that the parameters of the third-order method (2.12b) and fourth-order method (2.14b) and (2.14c) satisfy the conditions of theorem 2.4 and these methods have better results than the methods of the same order (2.11b) and (2.13b).

Table 3.2: NCD-values at $T = 20$ for problem (3.1) obtained by pth-order PTRK methods

Methods	w	p	$N_{steps} = 200$	$N_{steps} = 400$	$N_{steps} = 800$	$N_{steps} = 1600$	$N_{steps} = 3200$
PTRK (2.11b)	1	3	3.6	4.5	5.4	6.3	7.2
PTRK (2.12b)	1	3	4.5	5.4	6.3	7.2	8.1
PTRK (2.13b)	1	4	4.7	6.0	7.3	8.5	9.8
PTRK (2.14b)	2	4	6.1	7.3	8.6	9.8	11.0
PTRK (2.14c)	1	4	6.3	7.5	8.7	9.9	11.1

4 Concluding remarks

This paper proposed a new family of pseudo two-step RK methods. By a numerical test applied to a few methods from this family we showed the theoretical performance of the new methods. The approach considered in this paper can be applied for constructing more efficient pseudo two-step RK methods of arbitrarily high-order. In parallel PC iteration mode of these methods, the arbitrarily desired number of implicit stages for any order of accuracy is an attractive aspect for constructing the parallel PC methods with any desired number of processors depending on the curent computer systems even for sequential computers. In the forthcoming papers, we will pursue the study of pseudo two-step RK methods which involves with stability aspects, the optimal choice of the method parameters, efficient parallel PC iteration schemes with stepsize control.

Acknowledgement

A part of this work was done while I was a guest at the Institute of Numerical Mathematics, Halle University, Germany. I would like to thank Prof. Dr. K. Strehmel, Prof. Dr. R. Weiner for their hospitality and interest in my research.

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