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# Explicit Runge–Kutta–Nyström methods for the numerical solution of second order linear inhomogeneous IVPs

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Runge–Kutta–Nyström (RKN) methods for the numerical solution of inhomogeneous linear initial value problems with constant coefficients are considered.

A general procedure to construct explicit $s$-stage RKN methods with maximal order $p = s + 1$, similar to the developed by the authors (Montijano et al., 2023) for the class of second order IVP under consideration, depending on the nodes $c_i, i = 1, \dots, s$ is presented. This procedure requires only the solution of successive linear equations in the elements $a_{ij}$, $1 \le j < i \le s$ of the matrix of coefficients $\mathbf{A}$ of the RKN method and avoids the solution of non linear equations.

The remarkable fact is that using as free parameters the nodes $c_i, i = 1, \dots, s$ with a quadrature relation, the $s(s-1)/2$ elements of matrix $\mathbf{A}$ can be computed by solving successively linear systems with coefficients depending on the nodes, so that if they are non-singular we get a unique $s$-stage method with maximal order $s + 1$.

We obtain an optimized six-stage seventh-order RKN method in the sense that the nodes are chosen so that minimize the leading term of the local error. Finally, some numerical experiments are presented to test the behaviour of the optimized RKN method with others with Radau and Lobatto nodes.


## 1. Introduction

We consider second order Initial Value Problems (IVPs) for $d$-dimensional differential systems of second order linear inhomogeneous equations given by

$$\begin{aligned} &\frac{d^2y}{dt^2} = y''(t) = f(t, y) \equiv D\, y(t) + g(t), \qquad t \in [t_0, t_0 + T], \\ &y(t_0) = y_0 \in \mathbb{R}^d, \quad y'(t_0) = y'_0 \in \mathbb{R}^d, \end{aligned} \tag{1}$$

where $D \in \mathbb{R}^{d\times d}$ is a constant matrix and $g : \mathbb{R} \to \mathbb{R}^d$ is a sufficiently smooth function in the interval of interest.

We approximate the solution $y = y(t)$ of (1) and the derivative $y'(t)$ at $t = t_0 + h$ by means of an $s$-stage Runge–Kutta–Nyström (RKN) method given by

$$y_1 = y_0 + h\, y'_0 + h^2 \sum_{i=1}^{s} b_i^*\, K_i, \tag{2}$$

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$$y'_1 = y'_0 + h \sum_{i=1}^{s} b_i\, K_i, \tag{3}$$

where the stages $K_i \in \mathbb{R}^d$, $i = 1, \dots, s$ are defined by

$$K_i = f\left(t_0 + c_i\, h, y_0 + h\, c_i\, y'_0 + h^2 \sum_{j=1}^{s} a_{ij}\, K_j\right), \quad i = 1, \dots, s. \tag{4}$$

Here

$$c_i,\ b_i,\ b_i^*,\ a_{ij}, \quad i, j = 1, 2, \dots, s,$$

are real constants that define the method and for explicit methods $a_{ij} = 0$ for $s \geq j \geq i \geq 1$.

It is usual to specify the RKN method (2), (3), (4) by the Butcher tableau

$$\begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \mathbf{b}^{*T} \\ \hline & \mathbf{b}^T \end{array} \tag{5}$$

where

$$\mathbf{c} = (c_i) \in \mathbb{R}^s, \quad \mathbf{b} = (b_i) \in \mathbb{R}^s, \quad \mathbf{b}^* = \left(b_i^*\right) \in \mathbb{R}^s, \quad \mathbf{A} = \left(a_{ij}\right) \in \mathbb{R}^{s \times s}. \tag{6}$$

As remarked in [1] the derivation of special Runge–Kutta type methods for the second order equations $y'' = f(t, y)$ (usually referred to as RKN) attracted the attention of many researchers after the early paper of Nyström in 1925. An important reason is that this type of equations appear in many practical applications and further the direct approach is more efficient than the straightforward transformation of the second order equation in two first order equations. High order methods have been derived by Fehlberg [2] and Dormand et al. [3] and have been widely used for numerical integrators in many problems of Celestial Mechanics and other areas. For other applications related to semi discretizations of some partial differential equations special RKN methods have been proposed by Hoang [4]. In the derivation of particular methods the choice of the available parameters takes into account not only the accuracy but also linear stability properties related to the scalar test equation $y'' = -w^2 y$, $w > 0$ and several definitions have been proposed by van der Houwen [5] and Franco [6] that are considered for the derivation of particular methods. A more refined stability study of RKN methods has been given by Alonso et al. in [7] that consider as test equation the system $U'' + B^2\, U = f(t)$ where $B$ is symmetric positive definite matrix. Such a system allow to define a natural energy norm that can be used to give some general stability definitions. Also it is worth to remark the recent contributions of Simos and co-workers [8–11] that derive very efficient high order methods taking into account the local error and the stability properties.

The rest of the paper is organized as follows: In Section 2 the series expansion of the exact and numerical solution are studied. In Section 3 necessary and sufficient conditions for a given order are derived in a simple formulation. Some consequences of these conditions are remarked with particular emphasis such as the highest order of an $s$-stage method is $s + 1$ and also the relation with the quadrature rules and the simplifying conditions. In Sections 4 and 5 the derivation of particular families of $s$–stage methods with order $s + 1$ for $s = 3, 4$ is studied. In Section 6 it is shown that general $s$-stage methods with order $s + 1$ can be constructed by solving only linear systems. Here we follow the approach of the authors in [12] and in our opinion these procedure is a crucial step in the derivation of high order RKN methods. Moreover an optimized six-stage seventh-order RKN method in the sense that the nodes are chosen so that minimize the leading term of the local error and the dispersion and dissipation errors has been obtained. Finally in Section 7 some numerical experiments are presented to test the behaviour of the optimized RKN method with others sixth-stage, seventh-order RKN methods based on Radau and Lobatto nodes.

## 2. Series expansions of the exact and the numerical solutions

First of all we derive the series expansion of the exact solution $y(t)$ of (1) at $t = t_0 + h$ in powers of the step size $h$. The two matrix valued functions $\Phi_1(h)$ and $\Phi_2(h)$ that are the fundamental solutions of the homogeneous equation of (1), $y''(t) + Dy(t) = 0$ such that

$$\Phi_1(0) = I, \quad \Phi'_1(0) = 0, \ \text{and} \quad \Phi_2(0) = 0, \quad \Phi'_2(0) = I,$$

have the series expansions

$$\Phi_1(h) = \sum_{i\geq 0} \frac{h^{2i}}{(2i)!} D^i, \quad \Phi_2(h) = \sum_{i\geq 0} \frac{h^{2i+1}}{(2i+1)!} D^i, \tag{7}$$

and then the solution of the homogeneous of (1): $y(t_0 + h) = y_H(h)$ can be written as

$$y_H(h) = \Phi_1(h)\, y_0 + \Phi_2(h)\, y'_0. \tag{8}$$

The particular solution of (1): $y(t_0+h)=y_P(h)$ such that $y_P(0)=0,\ y_P'(0)=0$, is

$$y_P(h)=\int_0^h\left(\sum_{k\geq 0}\frac{(-1)^k(h-\tau)^{2k+1}}{(2k+1)!}\,D^k\right)\,g(t_0+\tau)\,\mathrm{d}\tau,$$

and substituting the Taylor expansion of $g(t_0+\tau)$ at $t_0$ and integrating we get

$$y_P(h)=\sum_{i,\,k\geq 0}\frac{h^{2k+2+i}}{(2k+i+2)!}\,D^k\,g_0^{(i)}, \tag{9}$$

where $g_0^{(i)}=\left.\dfrac{\mathrm{d}^i g(t)}{\mathrm{d}t^i}\right|_{t=t_0}$.

Then, the general solution of (1) is

$$y(t_0+h)=y_H(h)+y_P(h), \tag{10}$$

with $y_H$ and $y_P$ given by (8) and (9) respectively.

For the series expansion of the $s$-stage RKN method (2), (3), (4) we introduce some auxiliary notations

$$\mathcal{K}=\begin{pmatrix}K_1\\K_2\\\vdots\\K_s\end{pmatrix}\in\left(\mathbb{R}^d\right)^s,\quad \mathbf{e}=\begin{pmatrix}1\\1\\\vdots\\1\end{pmatrix}\in\mathbb{R}^s, \tag{11}$$

$$\omega^*_{k,\,j}=\mathbf{b}^{*T}\,\mathbf{A}^k\,\mathbf{c}^j,\quad \omega_{k,\,j}=\mathbf{b}^T\,\mathbf{A}^k\,\mathbf{c}^j,\quad j\geq 0,\ k\geq 0. \tag{12}$$

Also for $f:\mathbb{R}\to\mathbb{R}^d$ and $\mathbf{u}=(u_1,u_2,\ldots,u_s)^T\in\mathbb{R}^s$ we denote by $f(\mathbf{u})$ the $(d\times s)$-dim vector with components

$$f(\mathbf{u})=\begin{pmatrix}f(u_1)\\f(u_2)\\\vdots\\f(u_s)\end{pmatrix}\in\left(\mathbb{R}^d\right)^s. \tag{13}$$

With these notations, the Eqs. (2), (3) may be written as

$$y_1=y_0+h\,y_0'+h^2\,\left(\mathbf{b}^{*T}\otimes I_d\right)\,\mathcal{K}, \tag{14}$$

and

$$y_1'=y_0'+h\,\left(\mathbf{b}\otimes I_d\right)\,\mathcal{K}, \tag{15}$$

where $I_d$ is the identity matrix of order $d$ and $\otimes$ the standard Kronecker product and

$$\mathcal{K}=(\mathbf{e}\otimes D\,y_0)+h\,\left(\mathbf{c}\otimes D\,y_0'\right)+h^2\,\left(\mathbf{A}\otimes D\right)\,\mathcal{K}+g(t_0\,\mathbf{e}+h\,\mathbf{c}). \tag{16}$$

Then

$$\left[I_{ds}-h^2\,(\mathbf{A}\otimes D)\right]\,\mathcal{K}=(\mathbf{e}\otimes D\,y_0)+h\,\left(\mathbf{c}\otimes D\,y_0'\right)+g(t_0\,\mathbf{e}+h\,\mathbf{c}). \tag{17}$$

and taking into account that

$$\left[I_{ds}-h^2\,(\mathbf{A}\otimes D)\right]^{-1}=\sum_{j\geq 0}h^{2j}\,\left(\mathbf{A}\otimes D\right)^j,$$

and

$$g(t_0\mathbf{e}+h\mathbf{c})=(\mathbf{e}\otimes g_0)+\sum_{k\geq 1}\frac{h^k}{k!}\,(\mathbf{c}^k\otimes g_0^{(k)}),$$

we have

$$\begin{aligned}\left(\mathbf{b}^{*T}\otimes I_d\right)\,\mathcal{K}&=\left(\mathbf{b}^{*T}\otimes I_d\right)\,\left(\sum_{j\geq 0}h^{2j}\,\left(A\otimes D\right)^j\right)\\&\qquad\left[(\mathbf{e}\otimes D\,y_0)+h\,\left(\mathbf{c}\otimes D\,y_0'\right)+(\mathbf{e}\otimes g_0)+\sum_{k\geq 1}\frac{h^k}{k!}\,\mathbf{c}^k\otimes g_0^{(k)}\right]\\&=\sum_{j\geq 0}h^{2j}\,\omega^*_{0j}\,D^{j+1}\,y_0+\sum_{j\geq 0}h^{2j+1}\omega^*_{1j}\,D^{j+1}y_0'+\sum_{j,k\geq 0}\frac{h^{2j+k}}{k!}\,\omega^*_{kj}\,D^j g_0^{(k)}.\end{aligned}$$

In conclusion

$$y_1 = T_{N1} + T_{N2} + T_{N3}, \tag{18}$$

with

$$\begin{aligned} T_{N1} &= y_0 + \sum_{j\geq 0} h^{2j+2}\, \omega^*_{0j}\, D^{j+1}\, y_0, \\ T_{N2} &= h\, y'_0 + \sum_{j\geq 0} h^{2j+3}\, \omega^*_{1j}\, D^{j+1} y'_0, \\ T_{N3} &= \sum_{j,k\geq 0} \frac{h^{2j+k+2}}{k!}\, \omega^*_{kj}\, D^j g_0^{(k)}. \end{aligned} \tag{19}$$

Similarly for $y'_1$

$$y'_1 = y'_0 + h\, \left(\mathbf{b}^T \otimes I_d\right)\, \mathcal{K} = T'_{N1} + T'_{N2} + T'_{N3}, \tag{20}$$

with

$$\begin{aligned} T'_{N1} &= \sum_{j\geq 0} h^{2j+1}\, \omega_{0j}\, D^{j+1}\, y_0, \\ T'_{N2} &= y'_0 + \sum_{j\geq 0} h^{2j+2}\, \omega_{1j}\, D^{j+1} y'_0, \\ T'_{N3} &= \sum_{j,k\geq 0} \frac{h^{2j+k+1}}{k!}\, \omega_{kj}\, D^j g_0^{(k)}. \end{aligned} \tag{21}$$

## 3. Order conditions

Recall that a RKN method has order $p$ iff this is the largest positive integer such that

$$y(t_0+h) - y_1 = \mathcal{O}\left(h^{p+1}\right), \qquad y'(t_0+h) - y'_1 = \mathcal{O}\left(h^{p+1}\right), \tag{22}$$

hold for all second order IVP (1) under consideration. Then in view of the above expansions (18)–(21) of the exact and the RKN solutions we may state the following result

**Theorem 3.1.** *The RKN method (2), (3), (4) has order p if this is the largest positive integer such that the following conditions hold*

$$\omega^*_{k,j} := \mathbf{b}^{*T}\, \mathbf{A}^k\, \mathbf{c}^j = \frac{j!}{(2k+j+2)!}, \text{ for all } \quad k,j\geq 0 \quad \text{with} \quad 2k+j+2\leq p, \tag{23}$$

$$\omega_{k,j} := \mathbf{b}^{T}\, \mathbf{A}^k\, \mathbf{c}^j = \frac{j!}{(2k+j+1)!}, \text{ for all } \quad k,j\geq 0 \quad \text{with} \quad 2k+j+1\leq p. \tag{24}$$

### *3.1. Some consequences of Theorem 3.1*

**(1)** The order of a $s$-stage RKN method depends on the available parameters through the real constants $\omega_{i,k}$ and $\omega^*_{i,k}$. We suppose now, that $s = 2q+1$. Then, for a method with order $p \geq s+1$ the principal term of the local error ($PTLE$) of the RKN (18)–(20) is composed of the two terms

$$\begin{aligned} PTLE(y_0) &= h^{p+1}\, \left(\frac{1}{(p+1)!} - \omega^*_{q,0}\right) D^{q+1} y'_0 \\ &\quad + h^{p+1}\, \sum_{j=0}^{q} \left(\frac{1}{(p+1)!} - \frac{\omega^*_{j,p-2j-1}}{(p-2j-1)!}\right)\, D^j\, g_0^{(p-2j-1)}, \end{aligned} \tag{25}$$

and

$$\begin{aligned} PTLE(y'_0) &= h^{p+1}\, \left(\frac{1}{(p+1)!} - \omega_{q+1,0}\right) D^{q+2} y_0 \\ &\quad + h^{p+1}\, \sum_{j=0}^{q+1} \left(\frac{1}{(p+1)!} - \frac{\omega_{j,p-2j}}{(p-2j)!}\right)\, D^j\, g_0^{(p-2j)}, \end{aligned} \tag{26}$$

where the first terms of (25) and (26) are the contribution due to the homogeneous part of the solution and the second one to the non homogeneous part, both for the numerical solution and the first derivative respectively.

**(2)** The conditions (24) for $k = 0$, and $j = 0, 1, \ldots, p-1$

$$\mathbf{b}^T\,\mathbf{c}^j = \frac{1}{j+1}, \quad j = 0, 1, \ldots, p-1,$$

imply that the quadrature rule with the $s$ nodes $c_1, \ldots, c_s$ and weights $b_1, b_2, \ldots, b_s$ has degree of precision $\geq (p-1)$. Since the maximum degree of precision of a quadrature rule with $s$ nodes is $(2s-1)$ we have the necessary condition $p \leq 2s$ for any general RKN method (2), (3), (4) with $s$ stages.

**(3)** To compare the number of free parameters of an $s$-stage RKN method 5, (6) and the number of order conditions we observe that for a given positive integer $r$ the number of conditions $C_r$

$$\omega_{k,j} = \frac{j!}{(2k+j+1)!} \quad \text{with} \quad k, j \geq 0 \text{ and } \quad 0 \leq 2k+j \leq r,$$

is

$$C_r = \begin{cases} (q+1)^2, & \text{if } r = 2q, \\ (q+1)(q+2), & \text{if } r = 2q+1. \end{cases}$$

Hence the number of order conditions (23), (24) for even $p$ is

$$\text{NCon(Order}p) = C_{p-2}(\text{of } \omega^*) + C_{p-1}(\text{of } \omega) = \frac{p(p+1)}{2},$$

and similarly for odd $p$.

From this statement it follows that for any order $p$ the number of order conditions NCon(Order$p$) is $p(p+1)/2$.

On the other hand the number of free parameters of an $s$-stage RKN method is

$$\text{NFreePar}(s \text{ stages}) = s + s + s + \frac{s(s-1)}{2} = \frac{s(s+5)}{2}.$$

In view of the above for a RKN with $s$ stages we have

$$\begin{aligned} \text{NCon(Order}(s+2)) &= \frac{(s+2)(s+3)}{2} = \frac{s^2+5s+6}{2} \\ &> \frac{s^2+5s}{2} = \text{NFreePar}(s \text{ stages}) \end{aligned}$$

and therefore it is not expected that there exist RKN methods with $s$ stages and order $s+2$.

**(4)** For RKN with $s$ stages and order $s+1$ we have

$$\begin{aligned} \text{NCon(Order}(s+1)) &= \frac{(s+1)(s+2)}{2} = \frac{s^2+3s+2}{2}, \\ \text{NFreePar}(s \text{ stages}) &= \frac{s^2+5s}{2}. \end{aligned}$$

Hence

$$\text{NFreePar}(s \text{ stages}) - \text{NCon(Order}(s+1)) = s-1,$$

and we have an infinite set of methods depending on $(s-1)$ free parameters.

In particular, with three stages the maximum order will be $p = 4$ and there exists a two parameter family of RKN methods with three stages and order 4, and for four stages we expect to attain order 5 with three free parameters.

**(5) A relation between the weights b and b$^*$ of a non confluent $s$-stage RKN with order** $(s+1)$.

For an $s$-stage non-confluent RKN method of order $(s+1)$, i.e. with $c_i \neq c_j$ for all $i \neq j$, the vectors $\mathbf{b}$ and $\mathbf{b}^*$ satisfy

$$\mathbf{b}^* = \mathbf{b} - (\mathbf{b} \cdot \mathbf{c}). \tag{27}$$

Let $\boldsymbol{\Delta}$ be the $s$-dim vector $\boldsymbol{\Delta} = \mathbf{b}^* - \mathbf{b} + (\mathbf{b} \cdot \mathbf{c})$, then for all $s$-vectors $\mathbf{c}^j, j = 0, 1, \ldots, s-1$ we have

$$\boldsymbol{\Delta}^T\,\mathbf{c}^j = \mathbf{b}^{*T}\,\mathbf{c}^j - \mathbf{b}^T\,\mathbf{c}^j + (\mathbf{b}\cdot\mathbf{c})^T\,\mathbf{c}^j,$$

and taking into account the conditions (23) and (24) of Theorem 3.1 with $p = s+1$ we get

$$\boldsymbol{\Delta}^T\,\mathbf{c}^j = 0, \qquad j = 0, 1, \ldots, s-1,$$

and by the non confluence of the we have $\boldsymbol{\Delta} = \mathbf{0}$.

**(6) Order Conditions of a non confluent $s$-stage RKN for order $s+1$.**

In view of the relation (27) between $\mathbf{b}$ and $\mathbf{b}^*$ we may substitute the order conditions $\omega^*$ by other conditions that only involve the weight $\mathbf{b}$. Thus, for a non confluent $s$-stage RKN with order $(s+1)$ we have the equations

$$\mathbf{b}^T\,\mathbf{A}^K\mathbf{c}^j = \frac{j!}{(2k+j+1)!} \quad \text{for all } j,k \geq 0 \quad \text{with } 0 \leq 2k+j \leq s-1, \tag{28}$$

$$(\mathbf{b}\cdot\mathbf{c})^T\,\mathbf{A}^K\mathbf{c}^j = \frac{j!\,(2k+j+1)}{(2k+j+2)!} \quad \text{for all } j,k \geq 0 \quad \text{with } 0 \leq 2k+j \leq s-2. \tag{29}$$

**(7) A simplifying condition.**

The condition

$$\mathbf{A}\,\mathbf{e} = \frac{1}{2}\,\mathbf{c}^2, \tag{30}$$

has been considered by many authors [1] in the derivation of explicit RKN methods. For explicit methods (30) implies that $c_1 = 0$ and there are $(s-1)$ additional linear relations between the elements of the matrix $\mathbf{A}$.

On the other hand under the simplifying assumption (30) there are some order conditions of (23)–(24) that can be skipped

$$\begin{aligned} &\omega_{1,0},\ \omega_{2,0},\ \ldots,\omega_{k,0}, \quad \text{for} \quad 0 \leq 2k \leq p-1,\\ &\omega^*_{1,0},\ \omega^*_{2,0},\ldots,\omega^*_{k,0}, \quad \text{for} \quad 0 \leq 2k \leq p-2. \end{aligned} \tag{31}$$

Thus for order $p = s+1$ the simplifying assumption (30) introduces apart of $c_1 = 0$, $(s-1)$ additional linear relations between the elements of the matrix $\mathbf{A}$ and on the other hand there are $(s-1)$ order conditions (31) that can be skipped. This suggest that there is a close relation between the $s$-stage RKN methods with order $s+1$ with $c_1 = 0$ and those that satisfy the condition (30). In fact, we will show next that if the nodes satisfy some algebraic relation they are equivalent.

Let

$$\widehat{\boldsymbol{\Delta}} = \mathbf{A}\,\mathbf{e} - \frac{1}{2}\,\mathbf{c}^2, \tag{32}$$

and assume that a RKN method with $s = 2q$ stages and order $(s+1)$ (a similar proof holds for an odd number of stages). The method has order $p = s+1 = 2q+1$ and the order conditions are

$$\begin{aligned} \mathbf{b}^T\,\mathbf{A}^k\mathbf{c}^j &= \frac{j!}{(2k+j+1)!} \quad \text{for all } j,k \geq 0 \quad \text{with } 0 \leq 2k+j \leq 2q,\\ (\mathbf{b}^*)^T\,\mathbf{A}^k\mathbf{c}^j &= \frac{j!}{(2k+j+1)!} \quad \text{for all } j,k \geq 0 \quad \text{with } 0 \leq 2k+j \leq 2q-1. \end{aligned} \tag{33}$$

Then taking into account that $c_1 = 0$, we obtain

$$\mathbf{e}_1^T\,\widehat{\boldsymbol{\Delta}} = 0,$$

and by (33)

$$\mathbf{b}^T\widehat{\boldsymbol{\Delta}} = 0, \quad \mathbf{b}^T\mathbf{A}\,\widehat{\boldsymbol{\Delta}} = 0, \quad \ldots, \mathbf{b}^T\mathbf{A}^{q-1}\widehat{\boldsymbol{\Delta}} = 0.$$

Similarly for $\mathbf{b}^*$

$$(\mathbf{b}^*)^T\widehat{\boldsymbol{\Delta}} = 0, \quad (\mathbf{b}^*)^T\mathbf{A}\,\widehat{\boldsymbol{\Delta}} = 0, \ldots, (\mathbf{b}^*)^T\mathbf{A}^{q-2}\widehat{\boldsymbol{\Delta}} = 0.$$

This implies that the vector $\widehat{\boldsymbol{\Delta}}$ is orthogonal to the $s = 2q$ vectors

$$\mathbf{e}_1^T,\ \mathbf{b}^T,\ \mathbf{b}^T\mathbf{A},\ldots,\mathbf{b}^T\mathbf{A}^{(q-1)}, \quad (\mathbf{b}^*)^T, (\mathbf{b}^*)^T\mathbf{A},\ldots,(\mathbf{b}^*)^T\mathbf{A}^{(q-2)}. \tag{34}$$

Therefore if the vectors (34) are linearly independent, then $\widehat{\boldsymbol{\Delta}} = \mathbf{0}$ and the simplifying condition (32) is satisfied.

**(8) On the FSAL condition.**

In the practical derivation of explicit RK methods for first order equations it is usual to consider methods in which the last stage of a step coincides with the first stage of the next step. Such a condition that reduces the computational cost of a methods is usually referred to as FSAL. Next we consider explicit RKN methods with this condition, i.e. the last stage of the $s$-stage RKN in $[t_0, t_1 = t_0 + h]$ coincides with the first stage in $[t_1, t_2]$

$$K_{0,s} = K_{1,1}, \tag{35}$$

or else

$$\begin{aligned} f\Big(t_0 + c_s h, y_0 + h c_s y_0' + h^2 \sum_{j=1}^{s-1} a_{sj} K_{0,j}\Big) &= f(t_1 + c_1 h, y_1)\\ &= f\Big(t_1 + c_1 h, y_0 + h y_0' + h^2 \sum_{j=1}^{s} b_j^* K_{0,j}\Big). \end{aligned} \tag{36}$$

From the above equations it follows that the FSAL condition holds if and only if we have the following relations between the coefficients of the method

$$c_1 = 0,\ c_s = 1,\ a_{sj} = b_j^*,\ j = 1, \dots, s-1,\ \text{and } b_s^* = 0. \tag{37}$$

Note that the condition $b_s^* = 0$ follows from $c_s = 1$.

Since the $s$ stage explicit RKN methods for linear equations with maximal order $(s+1)$ depend on $(s-1)$ parameters one may wonder whether or not this freedom can be used to satisfy the FSAL conditions (37). The number of FSAL conditions in (37) are $(s + 1)$ and therefore we cannot expect that a maximal order method satisfies the FSAL condition. In fact for $s = 3$ it is straightforward to see that all methods with order 4 do not satisfy (37) with $s = 3$.

An alternative study would be to derive $s$-stage methods with order $s$ and the FSAL condition. Now we have the order conditions

$$\begin{aligned} \omega_{k,j}^* &= \frac{j!}{(2k+j+2)!}, \quad 2k+j+2 \le s, \\ \omega_{k,j} &= \frac{j!}{(2k+j+1)!}. \quad 2k+j+1 \le s. \end{aligned} \tag{38}$$

For non confluent nodes the $s$ equations

$$\omega_{0,j} = \mathbf{b}^T\ \mathbf{c}^j = \frac{1}{j+1}, \quad j = 0, \dots, s-1, \tag{39}$$

define uniquely $\mathbf{b} = (b_1, \dots, b_s)^T$ as function of the nodes.

Also from the $(s-1)$ equations

$$\omega_{0,j}^* = (\mathbf{b}^*)^T\ \mathbf{c}^j = \frac{j!}{(j+2)!}, \quad j = 0, \dots, s-2, \tag{40}$$

with $b_s^* = 0$ define uniquely $\mathbf{b}^* = (b_1^*, \dots, b_{s-1}^*, 0)^T$ as function of the nodes.

Now since $a_{sj} = b_j^*$ are given as function of the nodes we must determine the remaining $(s-1)(s-2)/2$ parameters $a_{ij}$ with $s-1 \ge i > j \ge 1$ of matrix $\mathbf{A}$ taking into account the conditions (38) with $k \ge 1$. There are $(s-1)(s-2)/2$ order conditions on the elements of $A$ to be satisfied i.e we have the same number of equations as parameters and a linearization process similar to [12] can be applied to solve such system so that except for an isolated set of values of the non confluent nodes there is a unique solution. In conclusion, for $s$-stage explicit RKN methods for linear equations with order $s$ there is a family of FSAL methods depending on $s-2$ parameters.

As an example we consider the case $s = 4$ methods with order $p = 4$. Taking $c_2$ and $c_3$ as free parameters we have for the other elements:

$$\begin{aligned} b_1 &= (1-2c_2-2c_3+6c_2c_3)/(12c_2c_3), \\ b_2 &= (2c_3-1)/(12(c_2-1)c_2(c_2-c_3)), \\ b_3 &= (2c_2-1)/(12(c_3-1)c_3(c_3-c_2)), \\ b_4 &= (3-4c_2-4c_3+6c_2c_3)/(12(c_2-1)(c_3-1)), \\ b_1^* &= (1-2c_2-2c_3+6c_2c_3)/(12c_2c_3), \\ b_2^* &= (2c_3-1)/(12c_2(c_2-c_3)), \\ b_3^* &= (2c_2-1)/(12c_3(c_3-c_2)), \\ b_3^* &= 0, \\ a_{21} &= c_2^2/2, \\ a_{31} &= (c_3(c_2^2(1-12c_3)+6c_2^3c_3-c_3^2+3c_2c_3(1+c_3)))/(6(c_2-1)c_2(2c_2-1)), \\ a_{32} &= c_3(c_2-c_3)(3c_2c_3-c_2-c_3)/(6(c_2-1)c_2(2c_2-1)). \end{aligned}$$

**(9)** The RKN method generated by a RK method for first order equations

Let $\widehat{\mathbf{c}}$, $\widehat{\mathbf{A}}$, $\widehat{\mathbf{b}}$ the Butcher coefficients of an $s$-stage RK method. When applied to the IVP

$$Y' = F(t, Y), \quad Y(t_0) = Y_0, \tag{41}$$

gives the approximation $Y_1 \simeq Y(t_0 + h)$ given by the equations

$$\begin{aligned} Y_1 &= Y_0 + h\sum_{i=1}^{s} \widehat{b}_i\, F_i, \\ F_i &= F(t_0 + \widehat{c}_i h, Y_0 + h\ \sum_{j=1}^{s} \widehat{a}_{ij} F_j). \quad i = 1, \dots, s. \end{aligned} \tag{42}$$

To apply this method (42) to the special second order equation

$$y'' = f(t, y), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \tag{43}$$

we transform (43) in a equivalent first order system putting

$$Y = \begin{pmatrix} y \\ y' \end{pmatrix}, \quad Y_0 = \begin{pmatrix} y_0 \\ y'_0 \end{pmatrix}, \quad F(t, Y) = \begin{pmatrix} y' \\ f(t, y) \end{pmatrix} = \begin{pmatrix} F^1 \\ F^2 \end{pmatrix}, \tag{44}$$

The application of (42) to (44) leads to

$$\begin{aligned} & y_1 = y_0 + h \ \textstyle\sum_{i=1}^s \widehat{b}_i \ F_i^1, \quad y'_1 = y'_0 + h \ \textstyle\sum_{i=1}^s \widehat{b}_i \ F_i^2, \\ & F_i^1 = y'_0 + h \textstyle\sum_{j=1}^s \widehat{a}_{ij} \ F_j^2, \quad F_i^2 = f(t_0 + \widehat{c}_i h, y_0 + h \textstyle\sum_{j=1}^s \widehat{a}_{ij} F_j^1), \end{aligned} \tag{45}$$

that are equivalent to

$$y_1 = y_0 + h \sum_i \widehat{b}_i \ y'_0 + h^2 \sum_{i,j} \widehat{b}_i \ \widehat{a}_{ij} \ F_j^2, \quad y'_1 = y'_0 + h \ \sum_i \widehat{b}_i \ F_i^2, \tag{46}$$

$$F_i^2 = f\left( t_0 + \widehat{c}_i h, y_0 + h \sum_j \widehat{a}_{ij} \ y'_0 + h^2 \sum_{j,k} \widehat{a}_{ij} \ \widehat{a}_{jk} \ F_j^2 \right).$$

Then it is equivalent to the $s$-stage RKN method with

$$c_j = \widehat{c}_j \quad c_i = \sum_j \widehat{a}_{ij}, \quad \sum_i \widehat{b}_i = 1, \quad b_i = \widehat{b}_i, \quad b_j^* = \sum_i \widehat{b}_i \widehat{a}_{ij}, \quad \mathbf{A} = \widehat{\mathbf{A}}^2. \tag{47}$$

For explicit methods $\widehat{\mathbf{A}}$ is lower triangular and then $\mathbf{A}$ has also zeros in the two main subdiagonals.

## 4. Three stage explicit RKN methods with order 4

According to (24) we have the six order conditions relatives to

$$\omega_{0,0}, \quad \omega_{0,1}, \quad \omega_{0,2}, \quad \omega_{0,3}, \quad \omega_{1,0}, \quad \omega_{1,1}, \tag{48}$$

and the four order conditions (23) relatives to $\omega^*$

$$\omega^*_{0,0}, \quad \omega^*_{0,1}, \quad \omega^*_{0,2}, \quad \omega^*_{1,0}. \tag{49}$$

To give an explicit derivation of fourth-order methods we propose the following approach:

From the conditions of $\omega_{0,0}$, $\omega_{0,1}$ and $\omega_{0,2}$ we obtain $b_1, b_2, b_3$ from the explicit equations

$$b_1 = \frac{2 - 3c_2 - 3c_3 + 6c_2c_3}{6(c_1 - c_2)(c_1 - c_3)}, \tag{50}$$

and $b_2, b_3$ by circular rotation $(1 \to 2, 2 \to 3, 3 \to 1)$.

Then substituting into

$$\omega_{0,3} = \mathbf{b}^T \ \mathbf{c}^3 = \frac{1}{4},$$

we get the condition on the nodes

$$-3 + 4c_2 + 4c_3 - 6c_2c_3 + 2c_1(2 - 3c_2 - 3c_3 + 6c_2c_3) = 0. \tag{51}$$

Also from $\omega^*_{0,0}$, $\omega^*_{0,1}$ and $\omega^*_{0,2}$ we get

$$b_1^* = \frac{1 - 2c_2 - 2c_3 + 6c_2c_3}{12(c_1 - c_2)(c_1 - c_3)}, \tag{52}$$

and $b_2^*$, $b_3^*$ by circular rotation $(1 \to 2, 2 \to 3, 3 \to 1)$.

And finally $\omega_{1,0}$, $\omega_{1,1}$ and $\omega^*_{1,0}$ are three linear equations in $a_{21}$, $a_{31}$ and $a_{32}$ that define these unknowns as functions of $\mathbf{b}$, $\mathbf{b}^*$ and $\mathbf{c}$ and also as functions of the nodes. For example

$$\begin{aligned} a_{21} &= \frac{(c_1 - c_2)(-c_2 - c_1 + 6c_1c_2)}{2(1 - 6c_1 + 6c_1^2)}, \\ a_{31} &= -\frac{b_2b_3 - 2\sqrt{3}b_3b_2^* - 4b_2b_3^* + 2\sqrt{3}b_2b_3^*}{24b_3(b_3b_2^* - b_2b_3^*)}, \\ a_{32} &= \frac{(-1 + 4c_1)(c_1 - c_3)(c_2 - c_3)}{4(c_1 - c_2)(2 - 3c_1 - 3c_2 + 6c_1c_2)}. \end{aligned} \tag{53}$$

In conclusion if the nodes $c_j$ satisfy (51) and $b_j^*, b_j, a_{jk}$ are well defined we have a three stage RKN method with order four. It is worth to note that for all set of nodes that satisfy (51) we cannot ensure that the linear system in the elements of $\mathbf{A}$, $a_{21}, a_{31}, a_{32}$ possess a solution. Thus with the choice

$$c_1 = \frac{3-\sqrt{3}}{6}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{3+\sqrt{3}}{6},$$

that satisfies (51), we have from (50) and (52)

$$\mathbf{b} = \frac{1}{2}(1, 0, 1)^T, \quad \mathbf{b}^* = \left(\frac{3+\sqrt{3}}{12}, 0, \frac{3-\sqrt{3}}{12}\right)^T,$$

and the system in $a_{21}, a_{31}, a_{32}$ has no solution.

A particular solution of (53) is the one given in Hairer [1]

$$\begin{aligned} &\mathbf{c} = (0, 1/2, 1)^T, \ \mathbf{b} = (1/6, 4/6, 1/6)^T, \ \mathbf{b}^* = (1/6, 1/3, 0)^T, \\ &a_{21} = 1/8, \quad a_{31} = 0, \quad a_{32} = 1/2. \end{aligned} \tag{54}$$

Another particular solution is the corresponding to the Gaussian nodes in [0, 1] given by

$$c_1 = \frac{1}{2} - \sqrt{\frac{3}{20}}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{1}{2} + \sqrt{\frac{3}{20}}.$$

Now

$$\mathbf{b} = \left(\frac{5}{18}, \frac{4}{9}, \frac{5}{18}\right)^T, \quad \mathbf{b}^* = \left(\frac{5+\sqrt{15}}{36}, \frac{2}{9}, \frac{5-\sqrt{15}}{36}\right)^T,$$

and the linear system in $a_{21}$, $a_{31}$ and $a_{32}$ has the unique solution

$$a_{21} = \frac{6-\sqrt{15}}{16}, \quad a_{31} = -\frac{3}{5} + \sqrt{\frac{3}{5}}, \quad a_{32} = \frac{6-\sqrt{15}}{10}.$$

Note that this three-stage fourth-order RKN has $\omega_{0,5} = 1/6$ and $\omega_{0,6} = 1/7$.

## 5. Four stage explicit RKN methods with order 5

According to (24) we have the nine order conditions relatives to of $\omega_{i,j}$

$$\begin{array}{lllll} \omega_{0,0}, & \omega_{0,1}, & \omega_{0,2}, & \omega_{0,3}, & \omega_{0,4}, \\ & & \omega_{1,0}, & \omega_{1,1}, & \omega_{1,2}, \\ & & & & \omega_{2,0}, \end{array} \tag{55}$$

and from (23) the six order conditions of $\omega^*$

$$\begin{array}{llll} \omega^*_{0,0}, & \omega^*_{0,1}, & \omega^*_{0,2}, & \omega^*_{0,3}, \\ & & \omega^*_{1,0}, & \omega^*_{1,1}. \end{array} \tag{56}$$

First of all we consider the equations $\omega_{0,0}$ to $\omega_{0,3}$ to obtain $b_1, b_2, b_3, b_4$ as a functions of the nodes $c_j$. Then we substitute into the equation of $\omega_{0,4}$, that is $\mathbf{b}^T\ \mathbf{c}^4 = 1/5$, obtaining the following non linear relation between the nodes

$$\begin{aligned} &(-12 + 15c_3 + 15c_4 - 20c_3c_4) + 5c_2(3 - 4c_3 - 4c_4 + 6c_3c_4) \\ &= 5c_1(-3 + 4c_3 + 4c_4 - 6c_3c_4 + 2c_2(2 - 3c_3 - 3c_4 + 6c_3c_4)). \end{aligned} \tag{57}$$

On the other hand from the equations

$$\omega^*_{0,0}, \quad \omega^*_{0,1}, \quad \omega^*_{0,2}, \quad \omega^*_{0,3},$$

we obtain $b_j^*, j = 1, 2, 3, 4$ depending on the nodes $c_i$.

There are still six equations to be satisfied (four in (55) and two in (56)) that will be used to determine the six elements in the matrix $\mathbf{A}$. All equations are linear in the elements $a_{ij}$ except the corresponding to $\omega_{2,0}$. However we may use the linearization process (see [12])to substitute this equation for another equivalent that is linear. In fact the equations of $\omega_{1,0}, \omega_{1,1}, \omega_{1,2}$ can be written in the matrix form

$$\mathbf{b}^T\ \mathbf{A}\ \left[\mathbf{e} \mid \mathbf{c} \mid \mathbf{c}^2\right] = (1/3!\ ,\ 1/4!,\ \ 2!/5!)\ ,$$

or else

$$\mathbf{b}^T\ \mathbf{A}\ \Omega_3 = \mathbf{b}^T\ \mathbf{A}\ \left[\mathbf{e} \mid \mathbf{c} \mid \mathbf{c}^2 \mid \mathbf{e}_4\right] = (1/3!\ ,\ 1/4!,\ \ 2!/5!\ ,\ 0) \equiv \mathbf{d}_1^T.$$

Hence

$$\mathbf{b}^T\,\mathbf{A} = \mathbf{d}_1^T\,\Omega_3^{-1} \equiv \boldsymbol{\mu}_1^T,$$

and then the second order equation in $\mathbf{A}$

$$\mathbf{b}^T\,\mathbf{A}^2\,\mathbf{e} = \frac{1}{5!},$$

can be substituted by

$$\boldsymbol{\mu}_1^T\,\mathbf{A}\,\mathbf{e} = \frac{1}{5!}. \tag{58}$$

Now the six equations $\omega_{1,0}$, $\omega_{1,1}$, $\omega_{1,2}$, (58), $\omega^*_{1,0}$, $\omega^*_{1,1}$ are linear equations that define $a_{ij}$.

In particular for $\mathbf{c} = (c_1, c_2, c_3, c_4)^T = (0, 1/5, 2/3, 1)^T$, the condition (57) is satisfied and we get the method defined by

$$\mathbf{b}^* = \left(\frac{14}{336}, \frac{100}{336}, \frac{54}{336}, 0\right)^T, \ \mathbf{b} = \left(\frac{14}{336}, \frac{125}{336}, \frac{162}{336}, \frac{35}{336}\right)^T,$$

$$\mathbf{A} = \begin{pmatrix} 0 & & & \\ 1/50 & 0 & & \\ -1/27 & 7/27 & 0 & \\ 3/10 & -2/35 & 9/35 & 0 \end{pmatrix},$$

given by Hairer et al. in [1].

## 6. The construction of explicit $s$-stage RKN linear methods of maximal order $s+1$.

An explicit $s$-stage RKN method for linear equations has $3s + s(s-1)/2$ parameters

$$\mathbf{c} = (c_i) \in \mathbb{R}^s, \quad \mathbf{b} = (b_i) \in \mathbb{R}^s, \quad \mathbf{b}^* = (b_i^*) \in \mathbb{R}^s, \quad \mathbf{A} = (a_{ij}),\ s \ge i > j \ge 1, \tag{59}$$

and for maximal order $p = s+1$ the order conditions are

$$\omega_{k,j} = \mathbf{b}^T\,\mathbf{A}^k\,\mathbf{c}^j = \frac{j!}{(2k+j+1)!} \equiv \gamma_{k,j}, \quad 0 \le 2k+j \le s, \tag{60}$$

$$\omega^*_{k,j} = \mathbf{b}^{*T}\,\mathbf{A}^k\,\mathbf{c}^j = \frac{j!}{(2k+j+2)!} \equiv \gamma^*_{k,j}, \quad 0 \le 2k+j \le s-1, \tag{61}$$

then there are $(s-1)$ free parameters.

After an elementary calculation it can be seen that the number of order conditions (60) and (61) are

$$\mathrm{NCond}_s = \frac{(s+1)(s+2)}{2},$$

and in these RKN methods with order $(s+1)$ there are $(s-1)$ free parameters.

To construct methods of maximal order we observe first that the conditions

$$\omega_{0,j} = \mathbf{b}^T\,\mathbf{c}^j = \frac{1}{j+1}, \quad j = 0, \ldots, s, \tag{62}$$

imply that the quadrature rule with nodes $c_j, j = 1, \ldots, s$ and weights $b_j, j = 1, \ldots, s$ has degree of precision $s$. The assuming non confluent nodes the first $s$ equations of (62) define uniquely the weights $b_i$, $i = 1, \ldots, s$ as rational functions of the nodes and we have the additional condition between the nodes

$$\mathbf{b}^T\,\mathbf{c}^s = \frac{1}{s+1}. \tag{63}$$

Moreover the order equations

$$\omega^*_{0,j} : \ (\mathbf{b}^*)^T\,\mathbf{c}^j = \frac{1}{(j+1)(j+2)}, \quad j = 0, \ldots, s-1, \tag{64}$$

define the weights $\mathbf{b}^{*T} = (b_1^*, \ldots, b_s^*)^T$ as functions of the nodes.

Now we must determine the $s(s-1)/2$ parameters $a_{ij}$ with $1 \le j < i \le s$ that define the matrix $\mathbf{A}$ from the $s(s-1)/2$ remaining order conditions of (59)–(60) with $\omega_{k,j}$ and $\omega^*_{k,j}$ with $k \ge 1$.

We have the same number of conditions as free parameters but the point here is that conditions $\omega_{i,j}$ and $\omega^*_{i,j}$ with $i \ge 2$ are non linear in the elements $a_{ij}$ of matrix $\mathbf{A}$.

The key point here is that the order conditions (59)–(60) with $k \ge 2$ are non linear in the elements of the matrix $\mathbf{A}$. However we will see that these non linear equations can be substituted by other equivalent linear equations in $a_{ij}$ and therefore the computation of $a_{ij}$ can be reduced to solve only linear systems with coefficients depending only on the nodes $c_j, j = 1, \dots, s$ and if these systems have a unique solution they will determine maximal order methods.

To fix ideas suppose that $s = 2q+1$ is an odd number (a similar study can be carried out for even $s$). Then, the $(2q+1)q$ equations that determine the $(2q+1)q$ elements of $\mathbf{A}$ are

$$\left\{ \begin{array}{l} \mathbf{b}^T\, \mathbf{A}\, \mathbf{c}^j = \gamma_{1,j}, \quad j = 0, 1, \dots, 2q-1, \\ \\ \mathbf{b}^{*T} \mathbf{A}\, \mathbf{c}^j = \gamma^*_{1,j}, \quad j = 0, 1, \dots, 2q-2, \end{array} \right. \tag{65}$$

$$\left\{ \begin{array}{l} \mathbf{b}^T\, \mathbf{A}^2\, \mathbf{c}^j = \gamma_{2,j}, \quad j = 0, 1, \dots, 2q-3, \\ \mathbf{b}^{*T} \mathbf{A}^2\, \mathbf{c}^j = \gamma^*_{2,j}, \quad j = 0, 1, \dots, 2q-4, \end{array} \right. \tag{66}$$

$$\vdots$$

$$\left\{ \begin{array}{l} \mathbf{b}^T\, \mathbf{A}^q\, \mathbf{c}^j = \gamma_{q,j}, \quad j = 0, 1, \\ \mathbf{b}^{*T} \mathbf{A}^q\, \mathbf{c}^j = \gamma^*_{q,j}, \quad j = 0. \end{array} \right. \tag{67}$$

where the first block (65) are linear equations in $\mathbf{A}$, the second block (66) are quadratic and the last block (67) have order $q$.

Now we consider the first set of $(s-1)$ equations of (65). Adding the identity $\mathbf{b}^T\, \mathbf{A}\mathbf{e}_s = 0$, these equations can be written equivalently in the matrix form

$$\mathbf{b}^T\, \mathbf{A} \left[\mathbf{e}|\mathbf{c}| \dots |\mathbf{c}^{s-2}|\mathbf{e}_s\right] = \left[\gamma_{0,1}, \dots, \gamma_{0,\,s-2}, \mathbf{b}^T\mathbf{A}\mathbf{e}_s = 0\right].$$

Therefore introducing the notations

$$\Omega_i = \left[\, \mathbf{e} \mid \mathbf{c} \mid \dots \mid \mathbf{c}^{i-1} \mid \mathbf{e}_{i+1} \mid \dots | \mathbf{e}_s \,\right] \in \mathbb{R}^{s\times s},$$
$$\overline{\boldsymbol{\gamma}}_i^T = (\gamma_{0,1}, \dots, \gamma_{0,\,i-1}, \mathbf{b}^T\mathbf{A}\mathbf{e}_{i+1}, \dots, \mathbf{b}^T\mathbf{A}\mathbf{e}_s), \quad i \le s-1,$$

the first equation of (65) can be written in the equivalent matrix form

$$\mathbf{b}^T\, \mathbf{A}\, \Omega_{2q} = \overline{\boldsymbol{\gamma}}_{2q}.$$

Next, we consider the second equation of (65), and adding the identities

$$\mathbf{b}^{*T}\mathbf{A}\mathbf{e}_s = 0, \quad \mathbf{b}^{*T}\mathbf{A}\mathbf{e}_{s-1} = \mathbf{b}^{*T}\mathbf{A}\mathbf{e}_{s-1},$$

and putting

$$\overline{\boldsymbol{\gamma}}_i^{*T} = \left(\gamma^*_{0,1}, \dots, \gamma^*_{0,\,i-2}, \mathbf{b}^{*T}\mathbf{A}\mathbf{e}_i, \dots, \mathbf{b}^{*T}\mathbf{A}\mathbf{e}_s\right),$$

can be written in the equivalent matrix form

$$\mathbf{b}^{*T}\, \mathbf{A}\, \Omega_{2q-1} = \overline{\boldsymbol{\gamma}}^*_{2q-1}.$$

These notations can be applied to (65)–(67) obtaining

$$\left\{ \begin{array}{l} \mathbf{b}^T\, \mathbf{A}\, \Omega_{2q} = \overline{\boldsymbol{\gamma}}_{2q}, \\ \mathbf{b}^{*T}\, \mathbf{A}\, \Omega_{2q-1} = \overline{\boldsymbol{\gamma}}^*_{2q-1}, \end{array} \right. \tag{68}$$

$$\vdots \quad \vdots$$

$$\left\{ \begin{array}{l} \mathbf{b}^T\, \mathbf{A}^q\, \Omega_2 = \overline{\boldsymbol{\gamma}}_2, \\ \mathbf{b}^{*T}\, \mathbf{A}^q\, \Omega_1 = \overline{\boldsymbol{\gamma}}^*_1. \end{array} \right. \tag{69}$$

Now defining

$$\begin{array}{ll} \boldsymbol{\mu}_1^T = \mathbf{b}^T\, \mathbf{A}, & \boldsymbol{\mu}_1^{*T} = \mathbf{b}^{*T}\, \mathbf{A}, \\ \boldsymbol{\mu}_2^T = \mathbf{b}^T\, \mathbf{A}^2 = \boldsymbol{\mu}_1^T\mathbf{A}, & \boldsymbol{\mu}_2^{*T} = \mathbf{b}^{*T}\, \mathbf{A}^2 = \boldsymbol{\mu}_1^{*T}\mathbf{A}, \\ \vdots & \vdots \\ \boldsymbol{\mu}_q^T = \mathbf{b}^T\, \mathbf{A}^q = \boldsymbol{\mu}_{q-1}^T\mathbf{A}, & \boldsymbol{\mu}_q^{*T} = \mathbf{b}^{*T}\, \mathbf{A}^q = {\boldsymbol{\mu}^*_{q-1}}^T\mathbf{A}, \end{array}$$

we have

$$\left\{ \begin{array}{l} \boldsymbol{\mu}_1^T\Omega_{2q} = \overline{\boldsymbol{\gamma}}_{2q} \to \boldsymbol{\mu}_1^T = \overline{\boldsymbol{\gamma}}_{2q}\Omega_{2q}^{-1}, \\ {\boldsymbol{\mu}^*}_1^T\Omega_{2q-1} = \overline{\boldsymbol{\gamma}}^*_{2q-1} \to {\boldsymbol{\mu}^*}_1^T = \overline{\boldsymbol{\gamma}}^*_{2q}\Omega_{2q-1}^{-1}, \end{array} \right. \tag{70}$$

$$\left\{ \begin{array}{l} \boldsymbol{\mu}_2^T\Omega_{2q-2} = \overline{\boldsymbol{\gamma}}_{2q-2} \to \boldsymbol{\mu}_2^T = \overline{\boldsymbol{\gamma}}_{2q-2}\Omega_{2q-2}^{-1}, \\ {\boldsymbol{\mu}^*}_2^T\Omega_{2q-3} = \overline{\boldsymbol{\gamma}}^*_{2q-3} \to {\boldsymbol{\mu}^*}_2^T = \overline{\boldsymbol{\gamma}}^*_{2q-3}\Omega_{2q-3}^{-1}, \end{array} \right. \tag{71}$$

$$
\vdots
$$

$$
\begin{cases} \boldsymbol{\mu}_q^T \boldsymbol{\Omega}_2 = \overline{\boldsymbol{\gamma}}_2 \to \boldsymbol{\mu}_q^T = \overline{\boldsymbol{\gamma}}_2 \boldsymbol{\Omega}_2^{-1}, \\ \boldsymbol{\mu}^{*T}_q \boldsymbol{\Omega}_1 = \overline{\boldsymbol{\gamma}}_1^* \to \boldsymbol{\mu}^{*T}_q = \overline{\boldsymbol{\gamma}}_1^* \boldsymbol{\Omega}_1^{-1}, \end{cases} \tag{72}
$$

Now the computation of the elements of **A** proceeds in the following way:

Solve for the $(s-1)$th-column of **A**, $a_{s\,s-1}$, from the $(s-1)$ component of $\mathbf{b}^T\ \mathbf{A} = \boldsymbol{\mu}_1^T$,

$$
b_s a_{s\,s-1} = \mu_{1,s-1},
$$

that defines $a_{s\,s-1}$ provided that $b_s \neq 0$.

Solve for the $(s-2)$th-column of **A**, i.e. from the $(s-2)$ components of $\mathbf{b}^T\ \mathbf{A} = \boldsymbol{\mu}_1^T$ and $\mathbf{b}^{*T}\ \mathbf{A} = \boldsymbol{\mu}_1^{*T}$, resulting the linear system $2 \times 2$

$$
\begin{pmatrix} b_s & b_{s-1} \\ b_s^* & b_{s-1}^* \end{pmatrix} \begin{pmatrix} a_{s,s-2} \\ a_{s-1,s-2} \end{pmatrix} = \begin{pmatrix} \mu_{1,s-2} \\ \mu_{1,s-2}^* \end{pmatrix}. \tag{73}
$$

Solve for the $(s-3)$th-column of **A**, i.e. from the $(s-3)$ components of $\mathbf{b}^T\ \mathbf{A} = \boldsymbol{\mu}_1^T$, $\mathbf{b}^{*T}\ \mathbf{A} = \boldsymbol{\mu}_1^{*T}$ and $\boldsymbol{\mu}_2^T\ \mathbf{A} = \boldsymbol{\mu}_1^T$ resulting the linear system $3 \times 3$

$$
\begin{pmatrix} b_s & b_{s-1} & b_{s-2} \\ b_s^* & b_{s-1}^* & b_{s-2}^* \\ 0 & \mu_{1,s-1} & \mu_{1,s-2} \end{pmatrix} \begin{pmatrix} a_{s,s-3} \\ a_{s-1,s-3} \\ a_{s-2,s-3} \end{pmatrix} = \begin{pmatrix} \mu_{1,s-3} \\ \mu_{1,s-3}^* \\ \mu_{2,s-3} \end{pmatrix},
$$

This process is repeated obtaining in the last step the linear system for the first column of **A**

$$
\begin{pmatrix} b_s & b_{s-1} & b_{s-2} & & \dots & b_2 \\ b_s^* & b_{s-1}^* & b_{s-2}^* & & \dots & b_2^* \\ 0 & \mu_{1,s-1} & \mu_{1,s-2} & & \dots & \mu_{1,2} \\ 0 & \mu_{1,s-1}^* & \mu_{1,s-2}^* & & \dots & \mu_{1,2}^* \\ \vdots & & & \ddots & & \\ 0 & \dots & 0 & \mu_{q-1,q+2} & \dots & \mu_{q-1,2} \\ 0 & \dots & 0 & \mu_{q-1,q+2}^* & \dots & \mu_{q-1,2}^* \end{pmatrix} \begin{pmatrix} a_{s\,1} \\ a_{s-1\,1} \\ a_{s-2\,1} \\ \\ \vdots \\ a_{3\,1} \\ a_{2\,1} \end{pmatrix} = \begin{pmatrix} \mu_{1,1} \\ \mu_{1,1}^* \\ \mu_{2,1} \\ \\ \vdots \\ \mu_{q,1} \\ \mu_{q,1}^* \end{pmatrix} \tag{74}
$$

Note that if the matrix in the linear system (74) is non singular, then it is possible to construct $s$-stages RKN methods with order $p = s+1$.

As remarked above the calculation of the $s(s-1)/2$ elements of the matrix **A** of an $s$-stage RKN method with order $p = s+1$ by solving only linear systems with coefficients $b_i$ depending on the nodes that satisfy the algebraic condition (63) can be carried out only if the successive linear systems to be solved in the above algorithm are non singular. Thus for $s = 3$, with the nodes $c_1 = (3-\sqrt{3})/6$, $c_2 = 1/2$, $c_3 = (3+\sqrt{3})/6$, the coefficients $b_1 = 1/2$, $b_2 = 0$, $b_3 = 1/2$ satisfy (62) and (63), but solving for the elements $a_{21}$ and $a_{31}$ of the first column of **A**, the coefficient matrix of (73) is singular, and then there is no solution for this set of nodes. Therefore apart of (63), there are additional algebraic conditions to be satisfied by the nodes to attain order $p = s+1$.

A particular interesting case is the closed Newton–Cotes nodes in $[0, 1]$ with an odd number of nodes $s = 2q+1$, $c_j = j/(2q)$, $j = 0, \dots, 2q$. In this case our numerical experiments show that for all $q$ there exist a unique $s$-stage method with maximal order $p = s+1$ with positive coefficients $b_i$ and $b_i^*$ and with the elements $a_{ij}$ given by rational numbers.

Thus for $s = 5$ we have the linear RKN method with

$$
\mathbf{c} = \left(0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1\right)^T, \quad \mathbf{b} = \left(\frac{7}{90}, \frac{16}{45}, \frac{2}{15}, \frac{16}{45}, \frac{7}{90}\right)^T, \mathbf{b}^* = \left(\frac{7}{90}, \frac{4}{15}, \frac{1}{15}, \frac{4}{15}, 0\right)^T,
$$

$$
A = \begin{pmatrix} 0 & & & & \\ 1/32 & 0 & & & \\ -1/24 & 1/6 & 0 & & \\ 5/32 & 1/8 & 1/16 & 0 & \\ 0 & 3/7 & -1/14 & 1/7 & 0 \end{pmatrix},
$$

that it has order 6. In Table 2 we give an five-stages sixth-order RKN method based on the nodes $\mathbf{c} = (1/5, 1/3, 1/2, 4/5, 2/3)^T$ and in Table 3 an seven-stage seventh-order FSAL RKN based on the nodes $\mathbf{c} = (0, 1/5, 1/4, 1/2, 2/3, 4/5, 1)^T$.

In relation with the choice of the $s-1$ free nodes in the $s$-stage explicit RKN methods with order $p = s+1$, we consider the minimization of the principal term of the local truncation error (25)–(26). Therefore, we take the Euclidean norm of the coefficients for the solution and their derivative. In the case that $s = 2q+1$,

$$
\mathbf{C}_{p+1}^T = \frac{1}{(p+1)!}(1, \dots, 1) - \left(\omega_{q,0}^*, \omega_{q,0}^*, \frac{\omega_{q-1,2}^*}{2!}, \dots, \frac{\omega_{1,p-4}^*}{(p-4)!}, \frac{\omega_{0,p-2}^*}{(p-2)!}\right) \in \mathbf{R}^{q+2},
$$

$$
\widehat{\mathbf{C}}_{p+1}^T = \frac{1}{(p+1)!}(1, \dots, 1) - \left(\omega_{q+1,0}, \omega_{q+1,0}, \frac{\omega_{q,2}}{2!}, \dots, \frac{\omega_{1,p-2}}{(p-2)!}, \frac{\omega_{0,p}}{p!}\right) \in \mathbf{R}^{q+3}.
$$

**Table 1**
Summary of six-stage seventh-order RKN methods.

| Method | $\|C_8\|$ | $\|\widehat{C}_8\|$ | $I_s$ | $\phi(\nu)$ | $d(\nu)$ |
|---|---|---|---|---|---|
| RKN6 new | $2.58 \times 10^{-7}$ | $2.25 \times 10^{-7}$ | 3.137 | $1.16 \times 10^{-7}\nu^9$ | $5.01 \times 10^{-10}\nu^8$ |
| Radau IA | $4.61 \times 10^{-7}$ | $4.15 \times 10^{-6}$ | 2.873 | $-8.44 \times 10^{-7}\nu^9$ | $1.56 \times 10^{-6}\nu^8$ |
| Lobatto IIIA | $1.36 \times 10^{-6}$ | $1.13 \times 10^{-6}$ | 3.131 | $-1.55 \times 10^{-7}\nu^9$ | $6.03 \times 10^{-7}\nu^8$ |

To study the absolute linear stability of an RKN method we consider the homogeneous linear test model [5]

$$y''(t) + \omega^2 y(t) = 0, \quad y(t_0) = y_0, \; y'(t_0) = y'_0, \quad \omega > 0, \tag{75}$$

whose analytical solution satisfies the relationship:

$$\begin{pmatrix} y(t_0+h) \\ y'(t_0+h)/\omega \end{pmatrix} = \begin{pmatrix} \cos(\nu) & \sin(\nu) \\ -\sin(\nu) & \cos(\nu) \end{pmatrix} \begin{pmatrix} y_0 \\ y'_0/\omega \end{pmatrix}$$

where $v = \omega h$. When an RKN method is applied to the above linear test IVP the following difference system is obtained:

$$\begin{pmatrix} y_1 \\ y'_1/\omega \end{pmatrix} = \mathbf{M}(\nu^2) \begin{pmatrix} y_0 \\ y'_0/\omega \end{pmatrix}, \quad \mathbf{M}(\nu^2) = \begin{pmatrix} m_{11}(\nu^2) & m_{12}(\nu^2) \\ -m_{21}(\nu^2) & m_{22}(\nu^2) \end{pmatrix}.$$

Here $\mathbf{M}(\nu^2)$ is the so called stability matrix whose elements are

$$\begin{aligned} m_{11}(\nu^2) &= 1 - \nu^2\, \mathbf{b}^{*T} \left(I + \nu^2 \mathbf{A}\right)^{-1} \mathbf{e}, & m_{12}(\nu^2) &= \nu - \nu^3\, \mathbf{b}^{*T} \left(I + \nu^2 \mathbf{A}\right)^{-1} \mathbf{c}, \\ m_{21}(\nu^2) &= \nu\, \mathbf{b}^T \left(I + \nu^2 \mathbf{A}\right)^{-1} \mathbf{e}, & m_{22}(\nu^2) &= 1 - \nu^2\, \mathbf{b}^T \left(I + \nu^2 \mathbf{A}\right)^{-1} \mathbf{c}. \end{aligned}$$

The behaviour of the numerical solution depends on spectral radius $\rho(\mathbf{M}(\nu^2))$. Then, for RKN methods, the stability interval is defined as $I_s = \{\nu > 0 \mid \rho(\mathbf{M}(\nu^2)) < 1\}$.

Once defined the stability matrix, a comparison between the numerical and exact solution of (75) leads to the following:

**Definition**

For an RKN method the dispersion error (phase error) and the dissipation error (amplification error) [5,6], are given respectively by

$$\phi(v) = v - \arccos\left[\frac{\operatorname{tr}\left(\mathbf{M}\left(v^2\right)\right)}{2\sqrt{\det\left(\mathbf{M}\left(v^2\right)\right)}}\right], \quad d(v) = 1 - \sqrt{\det\left(\mathbf{M}\left(v^2\right)\right)}.$$

Then the method is said to be dispersive of order $q$ and dissipative of order $r$, if

$$\phi(v) = \mathcal{O}\left(v^{q+1}\right), \quad d(v) = \mathcal{O}\left(v^{r+1}\right), \quad \nu \to 0.$$

To derive an optimized six-stage seventh-order RKN method with $c_1 = 0$, we select the free parameters $c_2, \ldots, c_5$ so that they minimize $\|\mathbf{C}_8\|^2 + \|\widehat{\mathbf{C}}_8\|^2$ with small values of the dispersive and dissipative errors. After this process of minimization, we obtain a rational set of values, rounding the optimized solution given by

$$\mathbf{c} = \left(0, \frac{3}{50}, \frac{9}{25}, \frac{11251}{12500}, \frac{18}{25}, \frac{24070733}{25588787}\right)^T.$$

The coefficients of this new method are given in Table 6 in Appendix.

We consider also a six-stage method obtained using the Lobatto IIIA ($c_1 = 0, c_6 = 1$) (see Table 4) and other scheme with the nodes of the RADAU IA quadrature nodes ($c_1 = 0$) (see Table 5). We present in Table 1 the main properties of the several RKN considered.

## 7. Numerical experiments

We present here some numerical experiments with the methods included in Table 1 and also the efficient six-stage, sixth-order FSAL DPRKN6 [3]. The Euclidean norm of all the coefficients of its *PTLE* is $3.99 \times 10^{-4}$.

We have considered the following test problems:

(I) Linear scalar inhomogeneous problem

$$y''(t) = -100y(t) + 99\sin(t), \quad y(0) = 1, \; y'(0) = 11, \; t \in [0, 20\pi],$$

with exact solution given by $y(t) = \cos(10t) + \sin(10t) + \sin(t)$. The step sizes used are $h = \dfrac{\pi}{5 \times 2^i}$, $i = 2, \ldots, 6$.

(II) Small dimensional linear system [7]

$$q''(t) = -\frac{1}{2}\begin{pmatrix} \omega^2+1 & \omega^2-1 \\ \omega^2-1 & \omega^2+1 \end{pmatrix} q(t), \quad q(0) = \begin{pmatrix} 1+\varepsilon \\ -1+\varepsilon \end{pmatrix}, \quad q'(0) = \begin{pmatrix} 1+\varepsilon\omega \\ -1+\varepsilon\omega \end{pmatrix},$$

whose analytic solution is given by

$$q(t) = \begin{pmatrix} \cos(t)+\sin(t) \\ -\cos(t)-\sin(t) \end{pmatrix} + \varepsilon \begin{pmatrix} \cos(\omega t)+\sin(\omega t) \\ \cos(\omega t)+\sin(\omega t) \end{pmatrix}$$

with $\varepsilon = 10^{-3}$, $\omega = 20$, and combines a dominant component of short frequency with a component of large frequency and small amplitude. In our test the problem is integrated up to $t_{\text{end}} = 20$ with steps $h = \dfrac{4\pi}{5 \times 2^i}$, $i = 2, \dots, 7$, and the numerical results obtained are presented in Fig. 2.

(III) Inhomogeneous linear system [8]

Starting from the wave equation given by

$$\begin{aligned} &\frac{\partial^2 x}{\partial t^2} = 4\frac{\partial^2 x}{\partial r^2} + \sin t \cdot \cos\left(\frac{\pi r}{L}\right), \qquad 0 \le r \le L, \quad t \in [0, 40\pi], \\ &\frac{\partial x}{\partial r}(t,0) = \frac{\partial x}{\partial r}(t,L) = 0, \\ &x(0,r) = 0,\ \frac{\partial x}{\partial t}(0,r) = \frac{L^2}{4\pi^2 - L^2}\cos\frac{\pi r}{L}, \end{aligned}$$

with exact solution

$$x(t,r) = \frac{L^2}{4\pi^2 - L^2} \cdot \sin(t) \cdot \cos\frac{\pi r}{L},$$

we semi-discretize $\frac{\partial^2 x}{\partial r^2}$ with fourth-order symmetric differences at internal points and one-sided differences of the same order at the boundaries obtaining the system:

$$\begin{bmatrix} x_1'' \\ x_2'' \\ x_{N+1}'' \end{bmatrix} = \frac{4}{(\Delta r)^2} \begin{bmatrix} -\frac{415}{72} & 8 & -3 & \frac{8}{9} & -\frac{1}{8} & 0 & \cdots & & \\ \frac{257}{144} & -\frac{10}{3} & \frac{7}{4} & -\frac{2}{9} & \frac{1}{48} & 0 & \cdots & & \\ -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & & & \vdots & \\ 0 & & \ddots & \ddots & \ddots & \ddots & \ddots & 0 & \\ \vdots & & & -\frac{1}{12} & \frac{4}{3} & -\frac{5}{2} & \frac{4}{3} & -\frac{1}{12} & \\ & \cdots & 0 & \frac{1}{48} & -\frac{2}{9} & \frac{7}{4} & -\frac{10}{3} & \frac{257}{144} & \\ & \cdots & 0 & -\frac{1}{8} & \frac{8}{9} & -3 & 8 & -\frac{415}{72} & \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{N+1} \end{bmatrix} + \sin t \cdot \begin{bmatrix} \cos\left(\frac{0\cdot\Delta r}{L}\cdot\pi\right) \\ \cos\left(\frac{1\cdot\Delta r}{L}\cdot\pi\right) \\ \vdots \\ \cos\left(\frac{N\cdot\Delta r}{L}\cdot\pi\right) \end{bmatrix}.$$

By choosing $L = 25$ and $N = 20$ and the spatial step size $\Delta r = L/N$, we arrive at a constant coefficient linear system. Then, $x_1 \approx x(t,0)$, $x_2 \approx x(t,\Delta r), \dots, x_{21} \approx u(t, 20\Delta r)$. The time step sizes used are $h = \dfrac{4\pi}{3 \times 2^i}$, $i = 2, \dots, 5$ and for computing the global error at each step, we have used the code DOPRI853 [1] at stringent tolerance after converting it in a first order IVP.

In Figs. 1, 2, 3 we show efficiency plots, computing the maximum global error ($\log_{10}(\max \|y(t_n) - y_n\|)$) over the whole integration interval and plotted against the number of required function evaluations.

From the numerical results obtained in Figs. 1, 2 and 3, it follows that for the problems under consideration, the efficiency of the RKN schemes developed for linear problems is clearly superior to the standard RKN scheme, being the optimized method deduced in the previous section the most efficient.

## 8. Conclusions

For the class of second-order linear inhomogeneous IVPs, the order conditions of explicit RKN methods have been obtained by a direct derivation without using the Butcher theory of $B$-series [13].

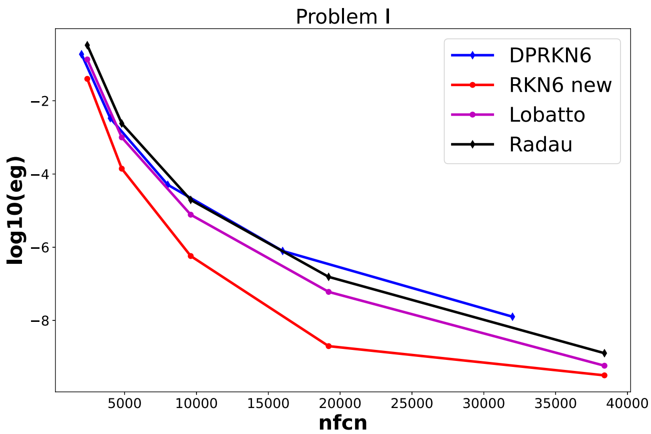


**Fig. 1.** Efficiency plot for problem I.

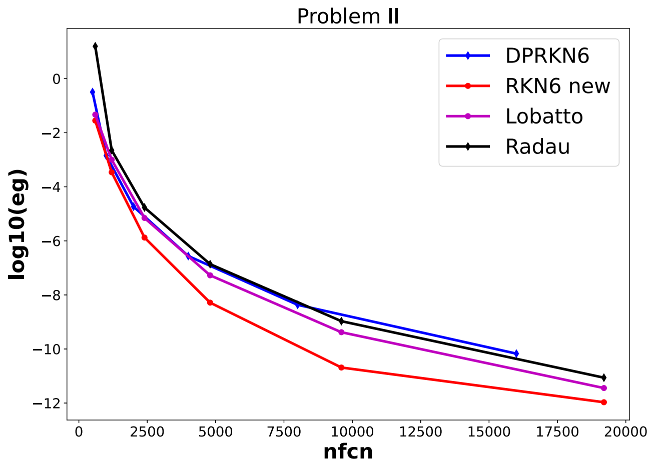


**Fig. 2.** Efficiency plot for problem II.

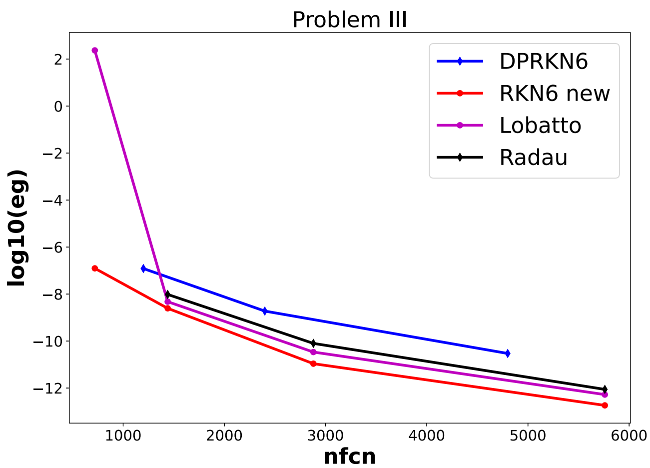


**Fig. 3.** Efficiency plot for problem III.

**Table 2**
Five-stage sixth-order RKN based on $c = (1/5, 1/3, 1/2, 4/5, 2/3)^T$.

| | | | | | |
|---|---|---|---|---|---|
| 1/5 | 0 | | | | |
| 1/3 | $\frac{8}{279}$ | 0 | | | |
| 1/2 | $\frac{7953}{63488}$ | $-\frac{15}{2048}$ | 0 | | |
| 4/5 | $\frac{369441}{1091200}$ | $-\frac{21819}{176000}$ | $\frac{168}{1375}$ | 0 | |
| 2/3 | $\frac{1560041}{8678016}$ | $\frac{811}{10368}$ | $-\frac{56}{2187}$ | $\frac{10}{2187}$ | 0 |
| $\mathbf{b}^{*T}$ | $\frac{275}{378}$ | $-\frac{27}{28}$ | $\frac{28}{27}$ | $\frac{275}{1512}$ | $-\frac{27}{56}$ |
| $\mathbf{b}^T$ | $\frac{1375}{1512}$ | $-\frac{81}{56}$ | $\frac{56}{27}$ | $\frac{1375}{1512}$ | $-\frac{81}{56}$ |

**Table 3**
Seven-stage seventh-order FSAL RKN.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 0 | 0 | | | | | | |
| $\frac{1}{5}$ | $\frac{1}{50}$ | 0 | | | | | |
| $\frac{1}{4}$ | $\frac{4814423}{73014272}$ | $-\frac{2532727}{73014272}$ | 0 | | | | |
| $\frac{1}{2}$ | $\frac{8765803965}{139813204096}$ | $-\frac{715410053}{139813204096}$ | $\frac{16525}{245104}$ | 0 | | | |
| $\frac{2}{3}$ | $\frac{83920581299}{4246826074416}$ | $-\frac{4192123959163}{12740478223248}$ | $\frac{4001725}{7445034}$ | $-\frac{35}{5832}$ | 0 | | |
| $\frac{4}{5}$ | $\frac{57110372996641}{2594190310375000}$ | $\frac{431735384596}{3631866434525}$ | $\frac{110480854}{1196796875}$ | $\frac{41283}{593750}$ | $\frac{1435401}{83125000}$ | 0 | |
| 1 | $\frac{29}{560}$ | $\frac{2125}{5292}$ | $-\frac{384}{1925}$ | $\frac{212}{945}$ | $-\frac{243}{4900}$ | $\frac{2375}{33264}$ | 0 |
| $\mathbf{b}^{*T}$ | $\frac{29}{560}$ | $\frac{2125}{5292}$ | $-\frac{384}{1925}$ | $\frac{212}{945}$ | $-\frac{243}{4900}$ | $\frac{2375}{33264}$ | 0 |
| $\mathbf{b}^T$ | $\frac{29}{560}$ | $\frac{10625}{21168}$ | $-\frac{512}{1925}$ | $\frac{424}{945}$ | $-\frac{729}{4900}$ | $\frac{11875}{33264}$ | $\frac{31}{560}$ |

The order conditions obtained do not assume the standard simplifying condition $\mathbf{Ae} = \mathbf{c}^2/2$.

By using the close connection of these order conditions with those which appear in the theory of degree of precision of quadrature rules, we have proposed an algorithm for the direct construction of $s$-stage explicit RKN methods that only requires the solution of linear systems in the elements $a_{ik}$, $s \geq i > k \geq 1$ of matrix $\mathbf{A}$.

Thus, our algorithm avoids the treatment of non-linear algebraic equations in the available parameters $a_{ik}$ by substituting these equations by equivalent linear equations obtained after suitable reduction.

Finally, the results of some numerical experiments to compare the behaviour of several 6-stages methods seventh-order RKN have been presented.

## Data availability

No data was used for the research described in the article.

## Acknowledgements

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## Appendix

See Tables 2–6.

**Table 4**
Six-stage seventh-order Lobatto IIIA RKN.

| |
|---|
| $a_{21}$ = 0.006899875101736095721792 |
| $a_{31}$ = −0.008649348384522627811526 |
| $a_{32}$ = 0.072511096513592418131778 |
| $a_{41}$ = 0.104494022647602567335994 |
| $a_{42}$ = −0.023548725703754618489262 |
| $a_{43}$ = 0.125532209425544389630595 |
| $a_{51}$ = −0.206831187509496682807197 |
| $a_{52}$ = 0.515997648211865580182855 |
| $a_{53}$ = −0.023154349324445859897361 |
| $a_{54}$ = 0.103415425688545404668997 |
| $a_{61}$ = 0.837331614754864935733926 |
| $a_{62}$ = −1.126061983315861349122818 |
| $a_{63}$ = 0.805147761593905739861816 |
| $a_{64}$ = −0.055588841946761896205889 |
| $a_{65}$ = 0.039171448913852569732965 |
| $b_1^*$ = 0.033333333333333333333333 |
| $b_2^*$ = 0.167007309146871573763622 |
| $b_3^*$ = 0.178280368337326917338981 |
| $b_4^*$ = 0.099148820180416259169378 |
| $b_5^*$ = 0.022230169002051916394684 |
| $b_6^*$ = 0 |
| $b_1$ = 0.033333333333333333333333 |
| $b_2$ = 0.189237478148923490158306 |
| $b_3$ = 0.277429188517743176508360 |
| $b_4$ = 0.277429188517743176508360 |
| $b_5$ = 0.189237478148923490158306 |
| $b_6$ = 0.033333333333333333333333 |
| $c_1$ = 0 |
| $c_2$ = 0.117472338035267653574498 |
| $c_3$ = 0.357384241759677451842924 |
| $c_4$ = 0.642615758240322548157075 |
| $c_5$ = 0.882527661964732346425501 |
| $c_6$ = 1 |

**Table 5**
Six-stage seventh-order Radau IA RKN.

| |
|---|
| $a_{21}$ = 0.0048545815666910426173870 |
| $a_{31}$ = 0.0178867174586194785795939 |
| $a_{32}$ = 0.0284842869433949608464863 |
| $a_{41}$ = −0.0085229470829495326182732 |
| $a_{42}$ = 0.0667757130306330902320682 |
| $a_{43}$ = 0.0996833910105472478290203 |
| $a_{51}$ = 0.0285399512356621006986177 |
| $a_{52}$ = 0.1971976976979077054873200 |
| $a_{53}$ = 0.0023568039193981549822464 |
| $a_{54}$ = 0.0934967861024179505405569 |
| $a_{61}$ = 0.0521153690477277501220434 |
| $a_{62}$ = −0.0094452871378897228108407 |
| $a_{63}$ = 0.3249664785174538438961446 |
| $a_{64}$ = 0.0502604721607108392479879 |
| $a_{65}$ = 0.0430855227197577349777399 |
| $b_1^*$ = 0.0277777777777777777777777 |
| $b_2^*$ = 0.1440724620885632070875976 |
| $b_3^*$ = 0.1687847241618682877292807 |
| $b_4^*$ = 0.1140764045101176825870768 |
| $b_5^*$ = 0.0412760290615843039880275 |
| $b_6^*$ = 0.0040126024000887408302394 |
| $b_1$ = 0.0277777777777777777777777 |
| $b_2$ = 0.1598203766102554832728899 |
| $b_3$ = 0.2426935942344849580799139 |
| $b_4$ = 0.2604633915947874912851147 |
| $b_5$ = 0.2084506671559538694797031 |
| $b_6$ = 0.1007941926267404201046003 |
| $c_1$ = 0 |
| $c_2$ = 0.0985350857988264261234988 |
| $c_3$ = 0.3045357266463639054853851 |
| $c_4$ = 0.5620251897526138559949874 |
| $c_5$ = 0.8019865821263918274642078 |
| $c_6$ = 0.9601901429485312576591933 |

**Table 6**
Six-stage seventh-order optimized RKN.

$$a_{21} = \frac{9}{5000}$$
$$a_{31} = -\frac{363406963788714007316}{53113189967339903376875}$$
$$a_{32} = \frac{566064347821661265291}{4249055197387192270150}$$
$$a_{41} = \frac{8054088664006320077374798453522968728624516971}{2255775205810430242066927075153523437500000000}$$
$$a_{42} = -\frac{15673554453785866571904623545471961034558496067}{3759625343017383736778211791922539062500000000}$$
$$a_{43} = \frac{66597022293443164742902591}{66361082082363281250000000}$$
$$a_{51} = \frac{2799906116457805865852985436372420713166301172318}{10683385770614357719482753057055174448979559399375}$$
$$a_{52} = -\frac{2030089456101085474684297666560587179060580676621}{9971223355899153000825561270299207793861377055625}$$
$$a_{53} = \frac{14957824304702535876353046357}{75433372650289261840211320625}$$
$$a_{54} = \frac{823529283413166000000}{339943616467082167731559}$$
$$a_{61} = \frac{3563203594163175979894004847721040446165535344779545910824501044838967229248444137}{5472003407206819031103218762906536765207466084551655581936948263663458130603102054}$$
$$a_{62} = -\frac{3925145090285808076404606818190932614058287091093530649340672243949908330338417695}{6242176849167648042166759522828558135927469310309664206886487432070529159127533566}$$
$$a_{63} = \frac{6834019611379007761629294570122746165710480958850239242171905}{19318392175580294085336879244732167995045801869596567299775309}$$
$$a_{64} = -\frac{16775559192347388888736811534232617978170556881875000000000}{504038350615804977199788645979977703459603971283672930280659}$$
$$a_{65} = \frac{235288433205605928365351457398836341141978199401775}{3378334474455160133475290334309091868500511394379014}$$

$$b_1^* = -\frac{46209807457411}{1579421172644856}$$
$$b_2^* = \frac{2112119288666500}{10542503391066999}$$
$$b_3^* = \frac{212185132357250}{914089036824459}$$
$$b_4^* = -\frac{3788196264648437500000000}{6993896944436859298543 4139}$$
$$b_5^* = \frac{1864640258070625}{20385839438418168}$$
$$b_6^* = \frac{39653947422209865160474257428271033679 7909}{36936271118274824682876038597998874219099636}$$
$$b_1 = -\frac{46209807457411}{1579421172644856}$$
$$b_2 = \frac{2246935413475000}{10542503391066999}$$
$$b_3 = \frac{2652314154465625}{7312712294595672}$$
$$b_4 = -\frac{3791229248046875000000000}{69938969444368592985434139}$$
$$b_5 = \frac{6659429493109375}{20385839438418168}$$
$$b_6 = \frac{401051509747134413752118142957442327783594 87}{221617626709648948097256231587993245314597816}$$
$$c = \left(0, \frac{3}{50}, \frac{9}{25}, \frac{11251}{12500}, \frac{18}{25}, \frac{24070733}{25588787}\right)^T$$

## References


[1] E. Hairer, S.P. Nørsett, G. Wanner, Solving Ordinary Differential Equations I: Nonstiff Problems, in: Springer Series in Computational Mathematics, Springer, Berlin, Heidelberg, 1993.
[2] E. Fehlberg, Eine Runge–Kutta-Nyström-Formel 9-ter Ordnung mit Schrittweitenkontrolle für Differentialgleichungen $\ddot{x} = f(t, x)$, ZAMM Z. Angew. Math. Mech. 61 (1981) 477–485.
[3] J.R. Dormand, M.E.A. El-Mikkawy, P.J. Prince, Families of Runge–Kutta-Nystrom formulae, IMA J. Numer. Anal. 7 (1987) 235–250.
[4] N.S. Hoang, Collocation Runge–Kutta-Nyström methods for solving second-order initial value problems, Int. J. Comput. Math. 98 (12) (2021) 2423–2444.
[5] P.J. van der Houwen, B.P. Sommeijer, Explicit Runge–Kutta (Nyström) methods with reduced phase errors for computing oscillating solutions, SIAM J. Numer. Anal. 24 (1987) 595–617.
[6] J.M. Franco, I. Gómez, Accuracy and linear stability of RKN methods for solving second-order stiff problems, Appl. Numer. Math. 59 (2009) 959–975.
[7] I. Alonso-Mallo, B. Cano, M.J. Moreta, Stability of Runge–Kutta-Nyström methods, J. Comput. Appl. Math. 189 (2006) 120–131.
[8] T.E. Simos, Ch. Tsitouras, Evolutionary derivation of Runge–Kutta pairs for addressing inhomogeneous linear problems, Numer. Algorithms 87 (2) (2020) 1–15.
[9] T.E. Simos, Ch. Tsitouras, On high order Runge–Kutta-Nyström pairs, J. Comput. Appl. Math. 400 (2022).
[10] V.N. Kovalnogov, R.V. Fedorov, M.T. Karpukhina, M.I. Kornilova, T.E. Simos, Ch. Tsitouras, Runge–Kutta-Nyström methods of eighth order for addressing Linear Inhomogeneous problems, J. Comput. Appl. Math. 419 (2023).
[11] Ch. Tsitouras, I.Th. Famelis, Symbolic derivation of Runge–Kutta-Nyström order conditions, J. Math. Chem. 46 (2009) 896–912.
[12] J.I. Montijano, L. Rández, M. Calvo, Explicit Runge–Kutta methods for the numerical solution of linear inhomogeneous IVPs, J. Comput. Appl. Math. 425 (2023).
[13] J.C. Butcher, Numerical Methods for Ordinary Differential Equations, John Wiley & Sons, 2003.