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1-PARAMETER FAMILIES OF MAXIMAL ORDER RUNGE-KUTTA-NYSTRÖM METHODS

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Abstract. Runge-Kutta-Nyström methods with s stages for the numerical solution of second order differential equations $d^2\mathbf{q}/dt^2 = \mathbf{f}(t, \mathbf{q})$ are considered. It is shown that the Gauss-Legendre schemes of order $2s$ consist of 1-parameter families involving an arbitrary constant. These schemes are symplectic and self-adjoint.

Key words. Runge-Kutta-Nyström, Gauss, Legendre, symplectic, symmetric, self-adjoint, symplectic integration

AMS(MOS) subject classifications. primary 65L06; secondary 70H05

1 Introduction

Consider the system of 2nd order ordinary differential equations

$$\frac{d^2}{dt^2}\,\mathbf{q} \;=\; \mathbf{f}(t, \mathbf{q})\,, \quad t \in \mathbb{R}\,, \quad \mathbf{q} \in \mathbb{R}^n \tag{1.1}$$

with some time-dependent vectorfield $\mathbf{f}(t, .) : \mathbb{R}^n \mapsto \mathbb{R}^n$. Numerical solutions of the initial value problem $\mathbf{q}(t_0) = \mathbf{q}_0$, $\frac{d\mathbf{q}}{dt}(t_0) = \mathbf{p}_0$ may be obtained by iterating the Runge-Kutta-Nyström (RKN) mapping $\Psi_h : (t_n, \mathbf{q}_n, \mathbf{p}_n) \mapsto (t_{n+1} = t_n + h, \mathbf{q}_{n+1}, \mathbf{p}_{n+1})$:

$$\begin{aligned} \mathbf{q}_{n+1} &= \mathbf{q}_n + h\,\mathbf{p}_n + h^2 \sum_{j=1}^{s} \bar{b}_j\,\mathbf{f}(t_n + c_j h, \mathbf{q}^{(j)})\,, \\ \mathbf{p}_{n+1} &= \mathbf{p}_n + h \sum_{j=1}^{s} b_j\,\mathbf{f}(t_n + c_j h, \mathbf{q}^{(j)}) \end{aligned} \tag{1.2}$$

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with the s **internal stages** $\mathbf{q}^{(i)}$ defined by the set of algebraic equations

$$\mathbf{q}^{(i)} = \mathbf{q}_n + h\,c_i\,\mathbf{p}_n + h^2 \sum_{j=1}^{s} A_{ij}\,\mathbf{f}(t_n + c_j h, \mathbf{q}^{(j)}) \;, \quad i = 1, \ldots, s \;. \tag{1.3}$$

The quantity h is the stepsize of the method which, upon a suitable choice of the parameters $(c_i, A_{ij}, \bar{b}_j, b_j)$, produces approximations $\mathbf{q}_n \approx \mathbf{q}(t_n)$, $\mathbf{p}_n \approx \frac{d\mathbf{q}}{dt}(t_n)$ of the exact solution $\mathbf{q}(t)$. Following [5] the parameters characterizing such a scheme are summarized in a **Butcher tableau:**

$$\begin{array}{c|ccc} c_1 & A_{11} & \ldots & A_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & A_{s1} & \ldots & A_{ss} \\ \hline & \bar{b}_1 & \ldots & \bar{b}_s \\ \hline & b_1 & \ldots & b_s \end{array} \tag{1.4}$$

The adjoint (reflected) map $\Psi_h^* := (\Psi_{-h})^{-1}$ is given by the RKN method (1.2)/(1.3) with parameters

$$c_i^* = 1 - c_i \;, \quad A_{ij}^* = A_{ij} + b_j - \bar{b}_j - c_i\,b_j \;, \quad \bar{b}_j^* = b_j - \bar{b}_j \;, \quad b_j^* = b_j$$

for $i, j = 1, \ldots, s$. A method is **self-adjoint** (or **symmetric**), if it is its own reflection. We note that a permutation of the RKN parameters only results in a permutation of the internal stages $\mathbf{q}^{(i)}$ without changing the mapping Ψ_h. Consequently, parameters satisfying the symmetry condition

$$c_{\sigma(i)} = 1 - c_i \;,\; A_{\sigma(i)\sigma(j)} = A_{ij} + b_j - \bar{b}_j - c_i\,b_j \;,\; \bar{b}_{\sigma(j)} = b_j - \bar{b}_j \;,\; b_{\sigma(j)} = b_j \;,$$

with some permutation $\sigma : \{1, \ldots, s\} \mapsto \{1, \ldots, s\}$ yield self-adjoint methods. Throughout this paper we fix

$$\bar{b}_j = b_j\,(1 - c_j) \;, \quad j = 1, \ldots, s \tag{1.5}$$

and refer to the parameters in (1.4) as (c_i, A_{ij}, b_j). This is a standard simplifying assumption leading to a significant reduction in the number of order equations which have to be satisfied by the parameters. It also simplifies the symmetry condition for self-adjoint methods to

$$c_{\sigma(i)} = 1 - c_i \;, \quad A_{\sigma(i)\sigma(j)} = A_{ij} + (c_j - c_i)\,b_j \;, \quad b_{\sigma(j)} = b_j \;, \tag{1.6}$$

with $i, j = 1, \ldots, s$. Further, Suris [12] showed that the RKN-method is symplectic when applied to a Hamiltonian system $d^2\,\mathbf{q}/dt^2 = -\nabla_{\mathbf{q}} V(\mathbf{q})$, if (1.5) holds together with

$$b_i\,A_{ij} - b_j\,A_{ji} = b_i\,b_j\,(c_i - c_j) \;, \quad i, j = 1, \ldots, s \;. \tag{1.7}$$

In the last decade much interest has been devoted to RKN methods, mostly in context with symplectic integration: for a survey and detailed references see, e.g., [9] or [10].

Most of this research is aimed at *explicit* methods (e.g., [2], [4], [7], [13]). In the following we shall consider *implicit* RKN methods of maximal order. For standard Runge-Kutta methods with s stages it is known that maximal order $2s$ can be attained [1, Section 343] with weights and abscissae corresponding to Gauss-Legendre quadrature. All parameters are fixed up to permutation. In [8] it was shown that corresponding RKN methods of order $2s$ may be constructed via collocation. However, this approach only leads to a subclass of methods and no parametric freedom was reported. We will show that in the Nyström case the methods of maximal order $2s$ are not unique, they admit one arbitrary parameter. Their construction is straightforward: weights and abscissae (b_j, c_j) are given by the Gauss-Legendre data, the matrix (A_{ij}) is determined by a *linear* system of simplifying equations with a 1-dimensional solution set. Finally, we list the resulting Butcher tableaus through $s = 5$ stages.

2 Order Theory

Following Hairer et al. [5] the conditions on the parameters (c_i, A_{ij}, b_j) to define a method of some specific order may be formulated via **special Nyström rooted trees** (sNr-trees) $\sigma\nu\rho\tau = [(V, E, r, \text{colour})]$. Here $V = \{1, \ldots, n\}$ is a set of labels for the vertices of the tree, $E \subset V \times V$ is the set of edges, $r \in V$ is the root and colour : $V \mapsto \{\text{black}, \text{white}\}$ is a colouring. The labeled representative (V, E, r, colour) gives rise to an equivalence class $[\,.\,]$ of trees which are equivalent under isomorphisms preserving adjacency of vertices and colour. The specification of the root $r \in V$ induces a direction on the edges (away from the root), whence edges $(i, j) \in E$ are given by ordered pairs of vertices $i, j \in V$ ("father" and "son"). Special Nyström trees have the properties: i) the root is black, ii) sons have different colours than their fathers, iii) a white vertex has at most 1 son. Vertices without sons shall be called **terminal**. For an sNr-tree $\sigma\nu\rho\tau$, given by a labeled representative (V, E, r, colour), we define

$$B = \{\, j \in V \ ;\ \text{colour}(j) = \text{black} \,\} \ , \quad W = \{\, j \in V \ ;\ \text{colour}(j) = \text{white} \,\} \ ,$$

$$BW = \{\, (i,j) \in E \ ;\ i \in B \ ,\ j \in W \ ,\ j \text{ is terminal} \,\} \ ,$$

$$BWB = \{\, (i,j,k) \in V \times V \times V \ ;\ (i,j) \in E \ ,\ (j,k) \in E \ ,\ i,k \in B \ ,\ j \in W \} \ .$$

The subset BW of E consists of all edges ●—○ with a white leaf, BWB represents the "double edges" ●—○—● consisting of black grandfathers/grandsons with a white father in between. Following [5] we define the RKN weights of a method (c_i, A_{ij}, b_j) by

$$\Phi(\sigma\nu\rho\tau) \ = \ \sum_{n_1=1}^{s} \sum_{n_2=1}^{s} \cdots \sum_{n_{|B|}=1}^{s} b_{n_r} \Big(\prod_{(i,j,k) \in BWB} A_{n_i n_k} \Big) \Big(\prod_{(i,j) \in BW} c_{n_i} \Big)$$

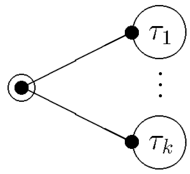
for an sNr-tree with root $r \in V$. The products are to be understood as 1, if either BWB or BW is empty, $|B|$ denotes the number of black vertices. The **density** γ of a rooted[1]

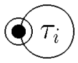
[1] In the pictorial representation the root is highlighted by a circle around the vertex.

tree is defined recursively [1, Section 144] by

$$\gamma(\odot) = 1 \ , \quad \gamma([\rho\tau_1, \ldots, \rho\tau_k]) = |\,[\rho\tau_1, \ldots, \rho\tau_k]\,|\; \gamma(\rho\tau_1)\,\gamma(\rho\tau_2)\cdots\gamma(\rho\tau_k) \ ,$$

where

$[\rho\tau_1, \ldots, \rho\tau_k] \ =$ 

is the grafting of the rooted trees $\rho\tau_i =$ 

onto a joint new root and $|\,.\,|$ denotes the number of vertices (i.e., $|[\rho\tau_1, \ldots, \rho\tau_k]| = 1 + |\rho\tau_1| + \cdots + |\rho\tau_k|$). The density ignores any colouring of the rooted tree. The order conditions of RKN methods are given by Hairer et al. [5, Theorem 13.12, Lemma 13.13]:

The RKN method (1.2)/(1.3)/(1.5) is of order N if and only if $\Phi(\sigma\nu\rho\tau) = 1/\gamma(\sigma\nu\rho\tau)$ for all sNr-trees $\sigma\nu\rho\tau$ through N vertices.

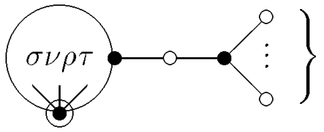
3 Gauss-Legendre Methods

Generalizing [5, Lemma 13.14] we observe

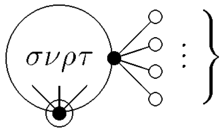
Lemma 3.1 *If*

$$\sum_{j=1}^{s} A_{ij}\, c_j^{k-1} = \frac{c_i^{k+1}}{k(k+1)} \ , \quad i = 1, \ldots, s \tag{3.8}$$

for some $k \in \mathbb{N}$, then $\Phi(\sigma\nu\rho\tau_1)\gamma(\sigma\nu\rho\tau_1) = \Phi(\sigma\nu\rho\tau_2)\gamma(\sigma\nu\rho\tau_2)$ for all sNr-trees of the form

$\sigma\nu\rho\tau_1 =$ 

$k-1$ terminal vertices

$\sigma\nu\rho\tau_2 =$ 

$k+1$ terminal vertices

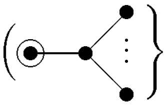
with the same (arbitrary) sNr-subtree $\sigma\nu\rho\tau$.

Proof The definition of the RKN weight yields

$$\Phi(\sigma\nu\rho\tau_1) = \sum_{i,j=1}^{s} (\cdots)_i\ A_{ij}\, c_j^{k-1} \ , \quad \Phi(\sigma\nu\rho\tau_2) = \sum_{i=1}^{s} (\cdots)_i\ c_i^{k+1} \ ,$$

where $(\cdots)_i$ represent terms associated with the edges in the joint subtree $\sigma\nu\rho\tau$. From (3.8) one concludes $\Phi(\sigma\nu\rho\tau_2) = k(k+1)\,\Phi(\sigma\nu\rho\tau_1)$. The recursive definition of the density yields

$$\gamma(\sigma\nu\rho\tau_1) = \gamma(\sigma\nu\rho\tau_2)\,\gamma\Big(\quad \Big\} \; k-1 \Big) \,,$$



i.e., $\gamma(\sigma\nu\rho\tau_1) = k(k+1)\,\gamma(\sigma\nu\rho\tau_2)$. □

Consequently, the order equations $\Phi(\sigma\nu\rho\tau)\,\gamma(\sigma\nu\rho\tau) = 1$ generated by the trees $\sigma\nu\rho\tau_1$ and $\sigma\nu\rho\tau_2$ coincide under the simplifying assumption (3.8).

For a given set of parameters (b_j, c_j) we consider a vector $(\alpha_1, \ldots, \alpha_s)$ spanning the kernel of the linear system

$$\text{(3.9)} \qquad \sum_{j=1}^{s} b_j\, c_j^{k-1} \alpha_j = 0 \;, \quad k = 1, \ldots, s-1 \;.$$

The corresponding $(s-1) \times s$-matrix $(b_j c_j^{k-1})$, $j = 1, \ldots, s$, $k = 1, \ldots, s-1$ is the product of a Vandermonde type matrix with entries $c_1, \ldots, c_s$ and $\mathrm{diag}(b_1, \ldots, b_s)$. For non-vanishing b_j and mutually distinct c_j the kernel is 1-dimensional, whence the vector (α_i) contains one arbitrary parameter. For an s-stage RKN scheme with parameters (c_i, A_{ij}, b_j) we introduce the statements

$$(A_{1\ldots s-1}): \quad \sum_{j=1}^{s} A_{ij}\, c_j^{k-1} = \frac{c_i^{k+1}}{k(k+1)} \,, \quad i = 1, \ldots, s \,, \quad k = 1, \ldots, s-1 \,,$$

$$(A_s): \quad \sum_{j=1}^{s} A_{ij}\, c_j^{s-1} = \frac{c_i^{s+1}}{s(s+1)} + \alpha_i \,, \quad i = 1, \ldots, s \,,$$

$$(B): \quad \sum_{j=1}^{s} b_j\, c_j^{k-1} = \frac{1}{k} \,, \quad k = 1, \ldots, 2s \,,$$

$$(C): \quad b_i\, A_{ij} - b_j\, A_{ji} = b_i\, b_j\, (c_i - c_j) \,, \quad i, j = 1, \ldots, s \,,$$

(D): the RKN scheme has order 2s.

The equations $(A_{1\ldots s-1})$ are the simplifying assumptions of lemma 3.1 which may be used to identify the order equations of trees $\sigma\nu\rho\tau_1$ with those of trees $\sigma\nu\rho\tau_2$ with "bushy subtrees" through s vertices. In conjunction with (A_s) these simplifying assumptions form a sufficiently large set of *linear* equations for the parameters A_{ij}, determining the matrix (A_{ij}) in terms of the parameters $(c_1, \ldots, c_s)$ and the arbitrary constant hidden in $(\alpha_1, \ldots, \alpha_s)$. The statement (B) represents the order conditions of the "bushy trees" (of height 1) through $2s$ vertices. It is well known (e.g., [1, Section 343]) that they fix $(c_1, \ldots, c_s)$ to be the distinct roots of a shifted Legendre polynomial on the interval $[0, 1]$.

The weights b_j are then expressed in terms of $(c_1, \ldots, c_s)$ by the set of linear equations (B) with $k = 1, \ldots, s$: they are the usual weights of Gaussian quadrature with abscissae $(c_1, \ldots, c_s)$. Thus, the conditions $(A_{1\ldots s-1})$, (A_s) and (B) fix all parameters (c_i, A_{ij}, b_j) up to a parametric freedom of one free constant represented by the vector $(\alpha_1, \ldots, \alpha_s)$. Together with the definition (1.5) one obtains the Gauss-Legendre-Nyström methods of order $2s$ which turn out to be symplectic (statement (C)):

Theorem 3.2

$$
\begin{aligned}
&\text{i)} & (A_{1\ldots s-1}),\ (A_s),\ (B) \ &\Rightarrow\ (C)\ ,\\
&\text{ii)} & (A_{1\ldots s-1}),\ (B),\ (C) \ &\Rightarrow\ (D)\ ,\\
&\text{iii)} & (A_{1\ldots s-1}),\ (A_s),\ (B) \ &\Rightarrow\ (D)\ .
\end{aligned}
$$

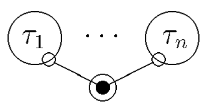
Proof i) For any $k, l \in \{1, \ldots, s\}$ the assumptions $(A_{1\ldots s-1})$ and (A_s) yield

$$
\sum_{i,j=1}^{s} c_i^{l-1}\ (\ b_i\, A_{ij} - b_j\, A_{ji} + b_i\, b_j\, (c_j - c_i)\ )\ c_j^{k-1} \ =
$$

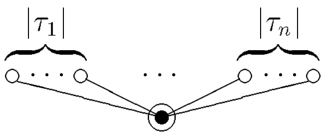
$$
\begin{aligned}
&\frac{1}{k(k+1)} \sum_{i=1}^{s} b_i\, c_i^{l+k} \ + \ \sum_{i=1}^{s} b_i\, c_i^{l-1}\, \alpha_i\, \delta_{ks} \ + \ \Big(\sum_{i=1}^{s} b_i\, c_i^{l-1}\Big)\Big(\sum_{j=1}^{s} b_j\, c_j^{k}\Big)\\
-\, &\frac{1}{l(l+1)} \sum_{j=1}^{s} b_j\, c_j^{l+k} \ - \ \sum_{j=1}^{s} b_j\, c_j^{k-1}\, \alpha_j\, \delta_{ls} \ - \ \Big(\sum_{i=1}^{s} b_i\, c_i^{l}\Big)\Big(\sum_{j=1}^{s} b_j\, c_j^{k-1}\Big)\ ,
\end{aligned}
$$

where δ denotes Kronecker's symbol. This expression vanishes for all $k, l = 1, \ldots, s$. Firstly, the two sums involving α_i are not present: they cancel for $k = l = s$, for $k = s, l = 1, \ldots, s-1$ (and $l = s, k = 1, \ldots, s-1$) each sum vanishes individually because of the conditions on $\alpha_1, \ldots, \alpha_s$. All remaining sums cancel trivially for $k = l = s$ and for $k + l < 2s$ after insertion of (B). As a consequence of (B) the abscissae $c_1, \ldots, c_s$ are distinct Legendre roots, whence the Vandermonde matrix (c_i^{l-1}) is invertible and (C) follows.

ii) Assuming that the scheme has order $N - 1 < 2s$ we show that it also has order N. In [3] it was shown that the order conditions of two root-shifted sNr-trees with N vertices coincide, if the order conditions of trees with less vertices are satisfied. With this simplifying principle one may shift the root in any sNr-tree with N vertices to a "central" black vertex minimizing the height. Consequently, only trees of the form



with sN-subtrees $\tau_1, \ldots, \tau_n$ of order $|\tau_i| \le \lfloor (N+1)/2 \rfloor \le s$ need to be considered. Recursive application of the simplifying principle of lemma 3.1 induced by $(A_{1\ldots s-1})$ allows to reduce any subtree with at most s vertices to a "bushy subtree" of height 1 with terminal white vertices directly linked to the root:



The order condition for the resulting sNr-tree of height 1 with $N \leq 2s$ vertices is satisfied by virtue of (B).

iii) clearly follows from i) and ii). □

Theorem 3.2 proves the existence of a 1-parameter family of s-stage RKN methods of order $2s$ defined by $(A_{1\ldots s-1})$, (A_s), (B) and (1.5):

i) The abscissae $c_1, \ldots, c_s$ are the distinct roots of the shifted Legendre polynomial $P_s(c) = \frac{d^s}{dc^s}\, c^s(1-c)^s$.

ii) The parameters $b_1, \ldots, b_s$ are the quadrature weights of Gaussian integration. They are determined by the set of linear equations

$$\sum_{j=1}^{s} b_j\, c_j^{k-1} = \frac{1}{k}\,, \quad k = 1, \ldots, s\,.$$

iii) The matrix (A_{ij}) is determined by the set of linear equations

$$\sum_{j=1}^{s} A_{ij}\, c_j^{k-1} = \frac{c_i^{k+1}}{k(k+1)} \;+\; \alpha_i\, \delta_{ks}\,, \quad i, k = 1, \ldots, s\,,$$

where $(\alpha_1, \ldots, \alpha_s)$ spans the 1-dimensional kernel of the linear system (3.9).

iv) The parameters $\bar{b}_1, \ldots, \bar{b}_s$ are given by (1.5).

According to theorem 3.2 all these schemes are symplectic for any value of the arbitrary parameter hidden in (α_i). Let us assume that the Legendre roots $c_1 < c_2 < \ldots < c_s$ are ordered, whence $c_{s+1-i} = 1 - c_i$, $i = 1, \ldots, s$. From the linear equations determining the other parameters it is easily checked that they feature the symmetry

$$A_{s+1-i,s+1-j} = A_{ij} + (c_j - c_i)\, b_j\,, \quad b_{s+1-i} = b_i\,, \quad i, j = 1, \ldots, s\,.$$

According to (1.6) with the permutation $\sigma(i) = s + 1 - i$ the Gauss-Legendre families are symmetric for any value of the arbitrary parameter.

Finally, the Butcher tableaus (1.4) through $s = 5$ stages are listed, they involve an arbitrary parameter α.

1 Stage, Order 2: The Butcher tableau

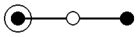
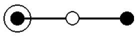
$$
\begin{array}{c|c}
1/2 & \alpha \\
\hline
 & 1/2 \\
\hline
 & 1
\end{array}
$$

yields the family of second order methods

$$
\mathbf{p}_{n+1} = \mathbf{p}_n + h\,\mathbf{f}(t_n + \frac{h}{2}, \mathbf{q}^{(1)}) \;, \quad \mathbf{q}_{n+1} = \mathbf{q}_n + \frac{h}{2}\,(\mathbf{p}_n + \mathbf{p}_{n+1})
$$

for (1.1) with the internal stage $\mathbf{q}^{(1)}$ determined by

$$
\mathbf{q}^{(1)} = \mathbf{q}_n + \frac{h}{2}\,\mathbf{p}_n + h^2\,\alpha\,\mathbf{f}(t_n + \frac{h}{2}, \mathbf{q}^{(1)}) \;.
$$

For $\alpha = 0$ one obtains the leap-frog method, the only explicit scheme in the Gauss-Legendre class. The principal error term of the family is minimized with $\alpha = 1/6$, which satisfies the order condition $\Phi($  $)\,\gamma($  $) = 1$ and leaves the only defect $1 - \Phi($  $)\,\gamma($  $) = 1/4$ at order 3.

2 Stages, Order 4:

$$
\begin{array}{c|cc}
\frac{1}{2} - \frac{\sqrt{3}}{6} & \alpha & -\alpha + \frac{1}{6} - \frac{\sqrt{3}}{12} \\
\frac{1}{2} + \frac{\sqrt{3}}{6} & -\alpha + \frac{1}{6} + \frac{\sqrt{3}}{12} & \alpha \\
\hline
 & \frac{1}{4} + \frac{\sqrt{3}}{12} & \frac{1}{4} - \frac{\sqrt{3}}{12} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

We note that for $\alpha = 1/6 \mp \sqrt{3}/12$ one obtains singly diagonally implicit schemes.

3 Stages, Order 6:

$$
\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & 4\,\alpha & -8\,\alpha+\frac{1}{10}-\frac{\sqrt{15}}{45} & 4\,\alpha+\frac{1}{10}-\frac{\sqrt{15}}{36} \\
\frac{1}{2} & -5\,\alpha+\frac{1}{16}+\frac{\sqrt{15}}{72} & 10\,\alpha & -5\,\alpha+\frac{1}{16}-\frac{\sqrt{15}}{72} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & 4\,\alpha+\frac{1}{10}+\frac{\sqrt{15}}{36} & -8\,\alpha+\frac{1}{10}+\frac{\sqrt{15}}{45} & 4\,\alpha \\
\hline
 & \frac{5+\sqrt{15}}{36} & \frac{2}{9} & \frac{5-\sqrt{15}}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

4 Stages, Order 8:

$$
\begin{array}{c|cccc}
c_1 & A_{11} & \left(S_{12}+\frac{c_1-c_2}{2}\right)b_2 & \left(S_{13}+\frac{c_1-c_3}{2}\right)b_2 & \left(S_{14}+\frac{c_1-c_4}{2}\right)b_1 \\
c_2 & \left(S_{12}+\frac{c_2-c_1}{2}\right)b_1 & A_{22} & \left(S_{23}+\frac{c_2-c_3}{2}\right)b_2 & \left(S_{13}+\frac{c_1-c_3}{2}\right)b_1 \\
c_3 & \left(S_{13}+\frac{c_3-c_1}{2}\right)b_1 & \left(S_{23}+\frac{c_3-c_2}{2}\right)b_2 & A_{22} & \left(S_{12}+\frac{c_1-c_2}{2}\right)b_1 \\
c_4 & \left(S_{14}+\frac{c_4-c_1}{2}\right)b_1 & \left(S_{13}+\frac{c_3-c_1}{2}\right)b_2 & \left(S_{12}+\frac{c_2-c_1}{2}\right)b_2 & A_{11} \\
\hline
 & b_1\,c_4 & b_2\,c_3 & b_2\,c_2 & b_1\,c_1 \\
\hline
 & b_1 & b_2 & b_2 & b_1
\end{array}
$$

with

$$
c_1=\frac{1}{2}-\frac{1}{70}\sqrt{525+70\sqrt{30}}\,,\quad c_3=\frac{1}{2}+\frac{1}{70}\sqrt{525-70\sqrt{30}}\,,
$$

$$
c_2=\frac{1}{2}-\frac{1}{70}\sqrt{525-70\sqrt{30}}\,,\quad c_4=\frac{1}{2}+\frac{1}{70}\sqrt{525+70\sqrt{30}}\,,
$$

$$
b_1=\frac{1}{4}-\frac{\sqrt{30}}{72}\,,\quad A_{11}=\frac{7\,\alpha\,(10-\sqrt{30})}{24}\,,
$$

$$
b_2=\frac{1}{4}+\frac{\sqrt{30}}{72}\,,\quad A_{22}=\frac{7\,\alpha\,(10+\sqrt{30})}{24}\,,
$$

$$
S_{12}=\frac{3}{14}-\left(\alpha+\frac{3}{490}\right)\sqrt{105}\,,\quad S_{14}=\left(\frac{9+\sqrt{30}}{1715}-\frac{\alpha}{7}\right)\left(75-4\sqrt{30}\right)\,,
$$

$$
S_{13}=\frac{3}{14}+\left(\alpha+\frac{3}{490}\right)\sqrt{105}\,,\quad S_{23}=\left(\frac{9-\sqrt{30}}{1715}-\frac{\alpha}{7}\right)\left(75+4\sqrt{30}\right)\,.
$$

5 Stages, Order 10:

$$
\begin{array}{c|ccccc}
c_1 & A_{11} & \left(S_{12}+\frac{c_1-c_2}{2}\right)b_2 & \left(S_{13}+\frac{c_1-c_3}{2}\right)b_3 & \left(S_{14}+\frac{c_1-c_4}{2}\right)b_2 & \left(S_{15}+\frac{c_1-c_5}{2}\right)b_1 \\
c_2 & \left(S_{12}+\frac{c_2-c_1}{2}\right)b_1 & A_{22} & \left(S_{23}+\frac{c_2-c_3}{2}\right)b_3 & \left(S_{24}+\frac{c_2-c_4}{2}\right)b_2 & \left(S_{14}+\frac{c_1-c_4}{2}\right)b_1 \\
c_3 & \left(S_{13}+\frac{c_3-c_1}{2}\right)b_1 & \left(S_{23}+\frac{c_3-c_2}{2}\right)b_2 & A_{33} & \left(S_{23}+\frac{c_2-c_3}{2}\right)b_2 & \left(S_{13}+\frac{c_1-c_3}{2}\right)b_1 \\
c_4 & \left(S_{14}+\frac{c_4-c_1}{2}\right)b_1 & \left(S_{24}+\frac{c_4-c_2}{2}\right)b_2 & \left(S_{23}+\frac{c_3-c_2}{2}\right)b_3 & A_{22} & \left(S_{12}+\frac{c_1-c_2}{2}\right)b_1 \\
c_5 & \left(S_{15}+\frac{c_5-c_1}{2}\right)b_1 & \left(S_{14}+\frac{c_4-c_1}{2}\right)b_2 & \left(S_{13}+\frac{c_3-c_1}{2}\right)b_3 & \left(S_{12}+\frac{c_2-c_1}{2}\right)b_2 & A_{11} \\
\hline
 & b_1\,c_5 & b_2\,c_4 & b_3\,c_3 & b_2\,c_2 & b_1\,c_1 \\
\hline
 & b_1 & b_2 & b_3 & b_2 & b_1
\end{array}
$$

with $c_3 = 1/2,\ b_3 = 64/225,\ A_{33} = \alpha$ and

$$
c_1 = \frac{1}{2} - \frac{1}{42}\sqrt{245 + 14\sqrt{70}}\,,\quad c_4 = \frac{1}{2} + \frac{1}{42}\sqrt{245 - 14\sqrt{70}}\,,
$$
$$
c_2 = \frac{1}{2} - \frac{1}{42}\sqrt{245 - 14\sqrt{70}}\,,\quad c_5 = \frac{1}{2} + \frac{1}{42}\sqrt{245 + 14\sqrt{70}}\,,
$$

$$
b_1 = \frac{161}{900} - \frac{13\sqrt{70}}{1800}\,,\quad A_{11} = \frac{2\,\alpha\,(14-\sqrt{70})}{63}\,,\quad S_{12} = \frac{5\,(55 - 3\sqrt{105})}{1134} - \frac{400\,\alpha}{189}\,,
$$
$$
b_2 = \frac{161}{900} + \frac{13\sqrt{70}}{1800}\,,\quad A_{22} = \frac{2\,\alpha\,(14+\sqrt{70})}{63}\,,\quad S_{14} = \frac{5\,(55 + 3\sqrt{105})}{1134} - \frac{400\,\alpha}{189}\,,
$$
$$
S_{13} = \frac{5\,(5\sqrt{70}-7)}{18144}\,(2\sqrt{70} + 5 + 240\,\alpha)\,,\quad S_{15} = \frac{5\,(257 - 10\sqrt{70})}{45927}\,(15 + \sqrt{70} + 80\,\alpha)\,,
$$
$$
S_{23} = \frac{5\,(5\sqrt{70}+7)}{18144}\,(2\sqrt{70} - 5 - 240\,\alpha)\,,\quad S_{24} = \frac{5\,(257 + 10\sqrt{70})}{45927}\,(15 - \sqrt{70} + 80\,\alpha)\,.
$$

4 Conclusions

We have given an explicit construction of the s-stage RKN schemes of maximal order $2s$. As in the general theory of Runge-Kutta methods the abscissae (c_i) and their weights (b_i) are the data of Gaussian quadrature. In the Nyström case the parameter matrix (A_{ij}) is not completely fixed by simplifying assumptions but has a parametric freedom of one arbitrary constant. All schemes feature the desirable properties of self-adjointness and symplecticity; they may serve as symplectic integrators for Hamiltonian systems. However, they are all implicit except for the leap-frog method, which probably makes them less efficient in practice than explicit symplectic methods of RKN type.

The combined attributes of self-adjointness and symplecticity enforce a certain symmetry on the parameters. In particular, with new parameters S_{ij} introduced by

$$
A_{ij} = \left(S_{ij} + \frac{c_i - c_j}{2}\right) b_j\ ,\quad i, j = 1, \ldots, s
$$

symplecticity (1.7) simplifies to the symmetry $S_{ij} = S_{ji}$ of the new parameter matrix. Self-adjointness corresponds to the symmetry with respect to reflection at the anti-diagonal $S_{s+1-i,s+1-j} = S_{ij}$ (see, e.g., the given Butcher tableaus for $s = 4$ and $s = 5$). Corresponding results were observed in [11] for standard Runge-Kutta methods. The modified order theory developed there may be adapted to the RKN case. Automatically reducing the order conditions to a smaller set of equations involving less parameters, it is more suitable for symplectic and self-adjoint schemes than the classical order theory of [5]. Details of this approach are presently under investigation [6].

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