MODIFIED ORDER THEORY FOR PARTITIONED RUNGE-KUTTA AND RUNGE-KUTTA-NYSTRÖM METHODS

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draft: version November 12, 1996

Abstract A parametrization technique for deriving general symplectic and/or self-adjoint (symmetric) Runge-Kutta methods of standard type was discussed in a recent paper by the authors. Here these results are extended to the derivation of order conditions for partitioned and Nyström-Runge-Kutta methods. These methods are of particular interest for the symplectic time-integration of Hamiltonian systems in separable form.

Key words. partitioned Runge-Kutta methods, Runge-Kutta-Nyström methods, symplectic, symmetric, self-adjoint, symplectic integration

AMS(MOS) subject classifications. primary 65L05; secondary 70H05

1 Introduction

The equations of motion for a conservative classical mechanical system with n degrees of freedom may be written as a set of $2n$ first order differential equations in Hamiltonian form:

$$\frac{d\mathbf{q}}{dt} = \nabla_{\mathbf{p}} H(\mathbf{q}, \mathbf{p}, t) \qquad , \qquad \frac{d\mathbf{p}}{dt} = -\nabla_{\mathbf{q}} H(\mathbf{q}, \mathbf{p}, t)\,. \tag{1.1}$$

The configuration coordinates and momenta $\mathbf{q}, \mathbf{p} \in \mathbf{R}^n$ together define the instantaneous state of the system and may be interpreted as the coordinates of a point in $\mathbf{R}^{2n} \times \mathbf{R}$, known as the (extended) *phase space* of the system. The scalar-valued Hamiltonian function $H(\mathbf{q}, \mathbf{p}, t) \in \mathrm{C}^1(\mathbf{R}^{2n} \times \mathbf{R})$ represents the total energy [12]. The derivation of numerical methods is simplified if we consider autonomous systems and there is no loss of generality in doing so.

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Many Hamiltonian problems of practical interest are of separable form:

$$H(\mathbf{q},\mathbf{p},t) = T(\mathbf{p},t) + V(\mathbf{q},t)\,, \tag{1.2}$$

where the term $V(\mathbf{q},t)$ is referred to as the potential energy. Most, but not all, of the problems of interest in this class involve an autonomous function of momenta (see for example [25] for a practical counter example). In particular, Newton's laws of motion can be modeled using a Hamiltonian system with the kinetic energy:

$$T(\mathbf{p},t) = \mathbf{p}^T\mathbf{p}/2 \tag{1.3}$$

and forces given by $-\nabla_{\mathbf{q}} V(\mathbf{q},t)$.

Ruth [15] first published symplectic methods for problems of the form (1.2). These methods were based on classical generating function techniques [9] and thus only applicable to Hamiltonian problems. The methods of Ruth have since been shown to be in direct correspondence with more established numerical techniques, variants of Runge-Kutta (RK) methods [17, 1, 14, 23].

In [22] Butcher's theory of order [2] for RK methods of standard type was re-designed, yielding a modified system of order constraints which is more appropriate for symplectic and/or self-adjoint implicit methods. The Butcher matrix is replaced by a new parameter matrix such that symplecticity and self-adjointness amount to simple symmetries among the new parameters. The structure of the modified order equations reflects such attributes in a very simple manner.

Here the results of [22] are extended to partitioned Runge-Kutta (pRK) methods and methods of Runge-Kutta-Nyström (RKN) type. In section 2 we give some definitions and a brief summary of the order formalism that will be of use later on. In section 3 the family of pRK methods is examined. This class encompasses explicit symplectic integrators for problems of the form (1.2). A new formulation of the order theory for such methods is presented. For the special case (1.3), equivalent to Newton's second order equations of motion, more efficient methods of RKN type are available. Their order theory is reformulated in section 4.

As for standard RK methods, in the new framework the attributes of symplecticity and self-adjointness correspond to linear constraints on the parameters of these methods. They may be satisfied identically by imposing simple symmetries among the parameters. Further, they serve as simplifying assumptions leading to a significant reduction of the complexity of the order conditions.

2 Bi-colour rooted trees and densities

Following Hairer et al. [10] the conditions on the parameters of pRK and RKN schemes to define a method of some specific order may be formulated via **bi-colour rooted trees** $\beta\rho\tau = [(V, E, r, \text{colour})]$. 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

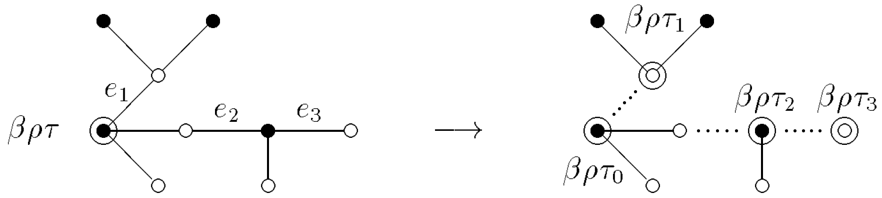


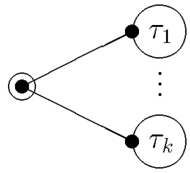
Table 1: Partitioning of $\beta\rho\tau$ by chopping $\{e_1, e_2, e_3\} \in C_3(\beta\rho\tau)$

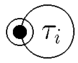
$[\,.\,]$ of trees which are equivalent under isomorphisms preserving adjacency of vertices and colour. The specification of the root $r \in V$ induces a direction on the edges (away from the root), whence edges $(i,j) \in E$ are given by ordered pairs of vertices $i, j \in V$ ("parent" and "child").

Certain combinatorial quantities on rooted trees play an important role in the order theory of Runge-Kutta type methods. The **density** γ of a rooted tree is defined recursively [2, 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 (in a pictorial representation the location of the root is indicated by a circle around the vertex). We use $|\,.\,|$ to denote 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.

In [22] it was demonstrated that a certain superposition of (reciprocal of) densities yields a useful combinatorial quantity in the theory of symplectic and self-adjoint RK schemes. We introduce the notion of partitions of a bi-colour rooted tree:

Definition 2.1 *A k-**partition** of a bi-colour rooted tree $\beta\rho\tau = [(V, E, r, \text{colour})]$ is a set of k mutually distinct edges $\{e_1, \ldots, e_k\} \subset E$. **Chopping** is the process of removing the edges of such a partition from $\beta\rho\tau$. In the removal of each edge the sub-tree containing the original root maintains its root. The remaining sub-tree is rooted at the vertex where the edge was chopped. The set of all k-partitions is denoted by $C_k(\beta\rho\tau)$, the bi-colour rooted sub-trees obtained by chopping the edges of a k-partition are denoted by $\beta\rho\tau_0, \ldots, \beta\rho\tau_k$.*

An illustration of this process is given in table 1. For non-coloured rooted trees $\rho\tau$ chopping results in a set of non-coloured rooted sub-trees $\rho\tau_0, \ldots, \rho\tau_k$. Following [22] we introduce:

Definition 2.2 *The* **modified reciprocal of density** *of a rooted tree $\rho\tau$ with $|E|$ edges is defined by*

$$\tilde{\delta}(\rho\tau) \;=\; \frac{1}{\gamma(\rho\tau)} \;+\; \sum_{k=1}^{|E|} \left(-\frac{1}{2}\right)^{k} \sum_{C_k(\rho\tau)} \frac{1}{\gamma(\rho\tau_0)} \cdots \frac{1}{\gamma(\rho\tau_k)} \;,$$

where the second sum extends over all $\binom{|E|}{k}$ k-partitions in $C_k(\rho\tau)$, each inducing a decomposition of $\rho\tau$ into the rooted sub-trees $\rho\tau_0, \ldots, \rho\tau_k$.

The main properties of $\tilde{\delta}$ are [22]:

Lemma 2.3

i) *$\tilde{\delta}$ changes its sign under root-shifting, i.e.,* $\tilde{\delta}\Big((\tau_1)\!\odot\!\!-\!\!\bullet(\tau_2)\Big) \;=\; -\;\tilde{\delta}\Big((\tau_1)\!\bullet\!\!-\!\!\odot(\tau_2)\Big)$ *for rooted trees with arbitrary sub-trees τ_1, τ_2.*

ii) *$\tilde{\delta}(\rho\tau) = 0$ for all rooted trees $\rho\tau$ with an even number of vertices.*

3 Partitioned Runge-Kutta methods

Consider dynamical systems

$$\frac{d}{dt}\begin{pmatrix} \mathbf{y} \\ \mathbf{Y} \end{pmatrix} \;=\; \begin{pmatrix} \mathbf{f}(\mathbf{y},\mathbf{Y}) \\ \mathbf{F}(\mathbf{y},\mathbf{Y}) \end{pmatrix}$$

with $\mathbf{y} \in \mathbb{R}^n$, $\mathbf{Y} \in \mathbb{R}^N$ and some vector fields $\mathbf{f} : \mathbb{R}^n \times \mathbb{R}^N \mapsto \mathbb{R}^n$, $\mathbf{F} : \mathbb{R}^n \times \mathbb{R}^N \mapsto \mathbb{R}^N$. Numerical solutions of the initial value problem $\mathbf{y}(t_0) = \mathbf{y}_0$, $\mathbf{Y}(t_0) = \mathbf{Y}_0$ may be obtained by iterating the pRK mapping $\Psi_h : (t_n, \mathbf{y}_n, \mathbf{Y}_n) \mapsto (t_{n+1} = t_n + h, \mathbf{y}_{n+1}, \mathbf{Y}_{n+1})$:

$$\begin{aligned} \mathbf{y}_{n+1} &= \mathbf{y}_n + h \sum_{j=1}^{s} b_j\, \mathbf{f}(\mathbf{y}^{(j)}, \mathbf{Y}^{(j)}) \;, \\ \mathbf{Y}_{n+1} &= \mathbf{y}_n + h \sum_{j=1}^{s} B_j\, \mathbf{F}(\mathbf{y}^{(j)}, \mathbf{Y}^{(j)}) \end{aligned} \tag{3.4}$$

with the internal stages $\mathbf{y}^{(i)}, \mathbf{Y}^{(i)}$ defined by the algebraic equations

$$\left.\begin{aligned} \mathbf{y}^{(i)} &= \mathbf{y}_n + h \sum_{j=1}^{s} a_{ij}\, \mathbf{f}(\mathbf{y}^{(j)}, \mathbf{Y}^{(j)}) \\ \mathbf{Y}^{(i)} &= \mathbf{Y}_n + h \sum_{j=1}^{s} A_{ij}\, \mathbf{F}(\mathbf{y}^{(j)}, \mathbf{Y}^{(j)}) \end{aligned}\right\} \quad i = 1, \ldots, s \;. \tag{3.5}$$

The quantity h is the stepsize of the method which, upon a suitable choice of the parameters $(a_{ij}, b_j, A_{ij}, B_j)$, produces approximations $\mathbf{y}_n \approx \mathbf{y}(t_n)$, $\mathbf{Y}_n \approx \mathbf{Y}(t_n)$ of the exact solution $(\mathbf{y}(t), \mathbf{Y}(t))$. In the following we assume non-vanishing weights (b_j, B_j) and replace the parameters (a_{ij}) and (A_{ij}) by new parameters (s_{ij}) and (S_{ij}), respectively, via

$$a_{ij} = \left(s_{ij} + \frac{1}{2}\right) b_j, \quad A_{ij} = \left(S_{ij} + \frac{1}{2}\right) B_j, \quad i,j = 1,\ldots,s \ . \tag{3.6}$$

As will become clear in the following subsections, this parametrization turns some useful properties of pRK schemes such as symplecticity and self-adjointness into a set of easily implementable *linear* constraints on the new parameters. Further, some of the order conditions become *homogeneous* equations.

It is worth noting that, since pRK methods effectively divide the dependent variables into two groups, quite different RK methods can be used for each of set of variables. For example, Sanz-Serna [18] suggests application to groups of stiff and non-stiff equations. However, this of little relevance in the context of symplecticity since the Hamiltonian nature rules out the existence of asymptotically stable attractors.

3.1 Self-adjoint pRK methods

The adjoint map $\Psi_h^* := (\Psi_{-h})^{-1}$ of the pRK scheme with parameters $(a_{ij}, b_j, A_{ij}, B_j)$ is given by the pRK scheme with parameters $(a_{ij}^*, b_j^*, A_{ij}^*, B_j^*)$:

$$a_{ij}^* = b_j - a_{ij} \ , \quad b_j^* = b_j \ , \quad A_{ij}^* = B_j - A_{ij} \ , \quad B_j^* = B_j \ , \quad i,j = 1,\ldots,s \ . \tag{3.7}$$

Self-adjoint methods are given by parameters satisfying the symmetry

$$a_{\pi(i)\pi(j)} = b_j - a_{ij} \ , \ b_{\pi(j)} = b_j \ , \ A_{\pi(i)\pi(j)} = B_j - A_{ij} \ , \ B_{\pi(j)} = B_j \ , \ i,j = 1,\ldots,s \ .$$

with some permutation $\pi : \{1,\ldots,s\} \mapsto \{1,\ldots,s\}$. This is a simple consequence of (3.7) in conjunction with the fact that any permutation of the parameters only permutes the internal stages in (3.5) without changing the mapping Ψ_h. In terms of the new parameters $(s_{ij}, b_j, S_{ij}, B_j)$ self-adjointness amounts to

$$s_{\pi(i)\pi(j)} = -s_{ij} \ , \ b_{\pi(j)} = b_j \ , \ S_{\pi(i)\pi(j)} = -S_{ij} \ , \ B_{\pi(j)} = B_j \ , \ i,j = 1,\ldots,s \tag{3.8}$$

with an arbitrary permutation π.

3.2 Symplectic pRK methods

Sanz-Serna [19] and Suris [24] independently showed (see also [1]) that the pRK scheme (3.4)/(3.5), $\mathbf{y} = \mathbf{q}$, $\mathbf{Y} = \mathbf{p}$, applied to a separable Hamiltonian system (1.1)/(1.2) defines a symplectic map Ψ_h if

$$b_i \, A_{ij} + B_j \, a_{ji} = b_i \, B_j \ , \quad i,j = 1,\ldots,s \ .$$

A proof of necessity can be found in [20, Section 6.5]. The symplecticity condition simplifies, without loss of generality for irreducible methods, to the *linear* constraint

$$S_{ij} = -s_{ji} \ , \quad i,j = 1,\ldots,s \tag{3.9}$$

on the new parameters introduced by (3.6). For non-separable Hamiltonian problems with a generic Hamiltonian $H(\mathbf{q}, \mathbf{p}, t)$ one also needs to impose the following conditions [16, 11]

$$b_j = B_j \ , \quad j = 1, \ldots, s \tag{3.10}$$

in order to obtain a symplectic method.

3.3 Order theory

Following Hairer et al. [10] the conditions on the pRK parameters to define a method of some specific order may be formulated via **pRK weights** associated with bi-colour rooted trees. For $\sigma\nu\rho\tau = [(V, E, r, \text{colour})]$ these weights are given by

$$\Phi_{pRK}(\beta\rho\tau) \ = \ \sum_{n_1=1}^{s} \cdots \sum_{n_{|V|}=1}^{s} B_{n_r} \ \Big(\prod_{\substack{(i,j)\in E \\ j\in W}} a_{n_i n_j} \Big) \Big(\prod_{\substack{(i,j)\in E \\ j\in B}} A_{n_i n_j} \Big) \ , \tag{3.11}$$

if the root r is black, and by

$$\Phi_{pRK}(\beta\rho\tau) \ = \ \sum_{n_1=1}^{s} \cdots \sum_{n_{|V|}=1}^{s} b_{n_r} \ \Big(\prod_{\substack{(i,j)\in E \\ j\in W}} a_{n_i n_j} \Big) \Big(\prod_{\substack{(i,j)\in E \\ j\in B}} A_{n_i n_j} \Big) \ , \tag{3.12}$$

if the root r is white. The sets $W \subset V$ and $B \subset V$ denote the white and black vertices, respectively, $|V|$ is the total number of vertices. The products are to be understood as 1, if the corresponding set of edges is empty. The order conditions of a pKN method are given by

[10, Section II.14]: *The pRK method (3.4)/(3.5) is of order N if and only if its parameters satisfy $\Phi_{pRK}(\beta\rho\tau) = 1/\gamma(\beta\rho\tau)$ for all bi-colour rooted trees $\beta\rho\tau$ through N vertices.*

In the application of pRK methods to separable problems

$$\frac{d}{dt} \begin{pmatrix} \mathbf{y} \\ \mathbf{Y} \end{pmatrix} \ = \ \begin{pmatrix} \mathbf{f}(\mathbf{Y}) \\ \mathbf{F}(\mathbf{y}) \end{pmatrix} \tag{3.13}$$

only **special bi-colour rooted trees** $\sigma\beta\rho\tau$ need to be considered. These are bi-colour rooted trees with the additional property:

- children have a different colour than their parent.

For such trees the colouring is fixed by the colour of the root. The conditions for a pRK method to be of order N when applied to separable dynamical systems (3.13) reduce to $\Phi_{pRK}(\sigma\beta\rho\tau) = 1/\gamma(\sigma\beta\rho\tau)$ for all special bi-colour rooted trees through N vertices.

3.4 Modified order conditions

Using the new parameters $(s_{ij}, b_j, S_{ij}, B_j)$ introduced by (3.6) we define the following modified weight:

Definition 3.1 *For a bi-colour rooted tree $\beta\rho\tau = [(V, E, r, \text{colour})]$ with $|V|$ vertices the* **modified pRK weight** *is defined by*

$$\tilde{\Phi}_{pRK}(\beta\rho\tau) \;=\; \sum_{n_1=1}^{s} \cdots \sum_{n_{|V|}=1}^{s} \Big(\prod_{\substack{(i,k)\in E \\ k\in W}} s_{n_i n_k} \Big) \Big(\prod_{k\in W} b_{n_k} \Big) \Big(\prod_{\substack{(i,k)\in E \\ k\in B}} S_{n_i n_k} \Big) \Big(\prod_{k\in B} B_{n_k} \Big) \, ,$$

where $W \subset V$ and $B \subset V$ denote the white and black vertices, respectively.

Pictorially, copies of the vectors $(b_j)/(B_j)$ are attached to the white/black vertices, copies of the matrices $(s_{ij})/(S_{ij})$ are attached to the edges with white/black children. The modified weights are polynomials in the new parameters $(s_{ij}, b_j, S_{ij}, B_j)$, which are obtained by replacing $a_{ij} \mapsto s_{ij} b_j$, $A_{ij} \mapsto S_{ij} B_j$ in the definitions (3.11)/(3.12) of the original pRK weights. Since the additive terms $b_j/2$ and $B_j/2$ in (3.6) are missing, the modified weights do not coincide with the original weights. They may be identified as polynomial expressions of the old weights as follows:

Lemma 3.2 *For any bi-colour rooted tree $\beta\rho\tau$ with $|E|$ edges:*

$$\tilde{\Phi}_{pRK}(\beta\rho\tau) \;=\; \Phi_{pRK}(\beta\rho\tau) \;+\; \sum_{k=1}^{|E|} \left(-\frac{1}{2}\right)^k \sum_{C_k(\beta\rho\tau)} \Phi_{pRK}(\beta\rho\tau_0) \cdots \Phi_{pRK}(\beta\rho\tau_k) \, ,$$

where C_k denotes the set of all $\binom{|E|}{k}$ k-partitions, each inducing a decomposition of $\beta\rho\tau$ into the bi-colour rooted sub-trees $\beta\rho\tau_0, \ldots, \beta\rho\tau_k$.

This result follows from formula (A.1) proven in the appendix. Comparing lemma 2.3 and definition 3.1 one sees that $\tilde{\Phi}_{pRK}$ and $\tilde{\delta}$ are obtained from Φ_{pRK} and $1/\gamma$ by the same deformation process. With

$$\begin{aligned} \tilde{\Phi}_{pRK}(\beta\rho\tau) - \tilde{\delta}(\beta\rho\tau) \;&=\; \Phi_{pRK}(\beta\rho\tau) - \frac{1}{\gamma(\beta\rho\tau)} \\ &+ \sum_{k=1}^{|E|} \left(-\frac{1}{2}\right)^k \sum_{C_k(\beta\rho\tau)} \left(\Phi_{pRK}(\beta\rho\tau_0) \cdots \Phi_{pRK}(\beta\rho\tau_k) - \frac{1}{\gamma(\beta\rho\tau_0) \cdots \gamma(\beta\rho\tau_k)} \right) \end{aligned} \tag{3.14}$$

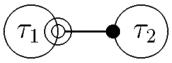
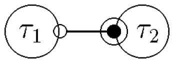
the old and new order condition for a bi-colour rooted tree coincide, provided the order conditions for lower order sub-trees are satisfied. Hence, induction on the number of vertices immediately leads to

Theorem 3.3 *The order conditions $\Phi_{pRK}(\beta\rho\tau) = 1/\gamma(\beta\rho\tau)$ for a pRK scheme are satisfied for all bi-colour rooted trees $\beta\rho\tau$ through N vertices if and only if $\tilde{\Phi}_{pRK}(\beta\rho\tau) = \tilde{\delta}(\beta\rho\tau)$ holds for all bi-colour rooted trees through N vertices.*

In the application of pRK methods to separable problems (3.13) the order conditions are given by *special* bi-colour rooted trees. Since chopping edges off such special trees leads to special bi-colour rooted sub-trees, one may again use (3.14) for an inductive proof of the equivalence of old and new order conditions:

Theorem 3.4 *For a pRK scheme applied to separable problems the order conditions $\Phi_{pRK}(\sigma\beta\rho\tau) = 1/\gamma(\sigma\beta\rho\tau)$ are satisfied for all special bi-colour rooted trees $\sigma\beta\rho\tau$ through N vertices if and only if $\tilde{\Phi}_{pRK}(\sigma\beta\rho\tau) = \tilde{\delta}(\sigma\beta\rho\tau)$ holds for all special bi-colour rooted trees through N vertices.*

In [1] it was observed the symplecticity of pRK schemes serves as a simplifying assumption relating the order conditions of root isomorphic trees. In terms of the new parameters one obtains

Theorem 3.5 *For symplectic pRK schemes the new order conditions $\tilde{\Phi}_{pRK}(\beta\rho\tau) = \tilde{\delta}(\beta\rho\tau)$ coincide for root-shifted trees $\beta\rho\tau_I =$  and $\beta\rho\tau_{II} =$  with arbitrary bi-colour sub-trees τ_1, τ_2.*

Proof Let $(V, E_I, r_I, \text{colour})$ and $(V, E_{II}, r_{II}, \text{colour})$ be labeled representatives of $\beta\rho\tau_I$ and $\beta\rho\tau_{II}$, respectively. With the edges $E_1, E_2 \subset V \times V$ of the sub-trees τ_1, τ_2 one has

$$E_I = E_1 \cup E_2 \cup \{(r_I, r_{II})\}\ , \quad E_{II} = E_1 \cup E_2 \cup \{(r_{II}, r_I)\}\ ,$$

whence all terms in definition 3.1 coincide for $\beta\rho\tau_I$ and $\beta\rho\tau_{II}$ apart from a single factor $s_{n_{r_I}, n_{r_{II}}}$ which has to be replaced by $S_{n_{r_{II}}, n_{r_I}}$. Symplecticity (3.9) yields $\tilde{\Phi}_{pRK}(\beta\rho\tau_I) = -\tilde{\Phi}_{pRK}(\beta\rho\tau_{II})$. With the root-shifting property of $\tilde{\delta}$ as stated in lemma 2.3.i) the new order equations remain unchanged when shifting the root between adjacent black and white vertices. □

For special bi-colour rooted trees adjacent pairs of vertices have different colours. Hence, the root may be shifted to *any* vertex in the tree, i.e., all rooted representatives of the same non-rooted special bi-colour tree give rise to the same new order condition:

Theorem 3.6 *A symplectic pRK schemes applied to a separable problem (3.13) is of order N if and only if the new order conditions $\tilde{\Phi}_{pRK}(\sigma\beta\rho\tau) = \tilde{\delta}(\sigma\beta\rho\tau)$ are satisfied by one rooted representative $\sigma\beta\rho\tau$ of every non-rooted special bi-colour tree through N vertices.*

This leads to a considerable reduction in the number of order conditions that have to be considered in the construction of symplectic pRK schemes [1]. Further, for self-adjoint schemes only order conditions associated with odd trees need to be considered:

Theorem 3.7 *For self-adjoint pRK schemes the new order conditions $\tilde{\Phi}_{pRK}(\beta\rho\tau) = \tilde{\delta}(\beta\rho\tau)$ are automatically satisfied for all bi-colour rooted trees $\beta\rho\tau$ with an even number of vertices.*

Proof With (3.8) re-summation $n_i \mapsto \pi(n_i)$, $i = 1, \ldots, |V|$, in definition 3.1 yields $\tilde{\Phi}_{pRK}(\beta\rho\tau) = (-1)^{|E|}\tilde{\Phi}_{pRK}(\beta\rho\tau)$ for a tree with $|E|$ edges. For an even number of vertices, i.e., odd $|E|$, one finds $\tilde{\Phi}_{pRK}(\beta\rho\tau) = 0$, matching the value of $\tilde{\delta}(\beta\rho\tau)$ according to lemma 2.3.ii). □

Remark 3.8 *In the new order framework the attributes of symplecticity (3.9) and self-adjointness (3.8) are easily implemented. The most interesting*[1] *permutation π leading to self-adjointness is $\pi(i) = s + 1 - i$. Any pRK method with parameters*

$$(3.15) \qquad (s_{ij}) = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \cdots & \cdots & \sigma_{1s} \\ -\sigma_{s-1,s} & \sigma_{22} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\sigma_{22} & \sigma_{s-1,s} \\ -\sigma_{1s} & \cdots & \cdots & -\sigma_{12} & -\sigma_{11} \end{pmatrix}, \quad (S_{ij}) = -(s_{ij})^T$$

and

$$(3.16) \qquad (b_j) = (b_1, b_2, \ldots, b_2, b_1), \quad (B_j) = (B_1, B_2, \ldots, B_2, B_1)$$

is both self-adjoint and symplectic, when applied to separable Hamiltonian systems. For general Hamiltonian systems (3.10) also has to be imposed for symplecticity. With

$$(3.17) \quad (s_{ij}) = \frac{1}{2}\begin{pmatrix} -1 & \cdots & \cdots & -1 \\ 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ 1 & \cdots & 1 & -1 \end{pmatrix}, \quad (S_{ij}) = \frac{1}{2}\begin{pmatrix} 1 & -1 & \cdots & -1 \\ \vdots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -1 \\ 1 & \cdots & \cdots & 1 \end{pmatrix}$$

one obtains a symplectic method consisting of an explicit and a diagonally implicit subprocess. It yields an explicit method when applied to separable problems (c.f. [20, Section 6.4]).

The number of free parameters for a general s-stage pRK method is $2\,s(s+1)$. For a symplectic method under the parametrization (3.6)/(3.9) this reduces to $s(s+2)$ free parameters. For the most general symplectic self-adjoint pRK method (3.15)/(3.16) the number of free parameters is $\lfloor (s+1)^2/2 \rfloor$, where $\lfloor x \rfloor$ denotes the integer part of x. An explicit symplectic pRK method (3.17) is prescribed by $2\,s$ free parameters $b_1, \ldots, b_s$, $B_1, \ldots, B_s$. With (3.16) the most general explicit self-adjoint pRK method is prescribed by $2\,\lfloor (s+1)/2 \rfloor$ free parameters.

[1] The row-sums $\tilde{c}_i = \sum_j s_{ij}\, b_j$, $\tilde{C}_i = \sum_j S_{ij}\, B_j$ satisfy $\tilde{c}_{\pi(i)} = -\tilde{c}_i$, $\tilde{C}_{\pi(i)} = -\tilde{C}_i$. Any fixed point i^* of the permutation leads to $\tilde{c}_{i^*} = \tilde{C}_{i^*} = 0$. Any orbit of π of length > 2 leads to coinciding values for some of the row-sums: $\tilde{c}_i = -\tilde{c}_{\pi(i)} = \tilde{c}_{\pi(\pi(i))} = \ldots$ etc. Such degeneracy does not occur for $\pi(i) = s+1-i$: all orbits are of length 2 apart from a single fixed point (for odd s).

4 Runge-Kutta-Nyström methods

Consider the system of 2nd order differential equations

$$\frac{d^2}{dt^2}\,\mathbf{q} \;=\; \mathbf{F}(t,\mathbf{q})\ , \quad t\in\mathbb{R}\ , \quad \mathbf{q}\in\mathbb{R}^n \tag{4.18}$$

with some time-dependent vector field $\mathbf{F}(t,.) : \mathbb{R}^n \mapsto \mathbb{R}^n$. 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 RKN mapping $\Psi_h : (t_n, \mathbf{q}_n, \mathbf{p}_n) \mapsto (t_{n+1} = t_n + h, \mathbf{q}_{n+1}, \mathbf{p}_{n+1})$:

$$\begin{aligned} \mathbf{q}_{n+1} &= \mathbf{q}_n + h\,\mathbf{p}_n + h^2 \sum_{j=1}^{s} \beta_j\,\mathbf{F}(t_n + c_j h, \mathbf{q}^{(j)})\ , \\ \mathbf{p}_{n+1} &= \mathbf{p}_n + h \sum_{j=1}^{s} B_j\,\mathbf{F}(t_n + c_j h, \mathbf{q}^{(j)}) \end{aligned} \tag{4.19}$$

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

$$\mathbf{q}^{(i)} = \mathbf{q}_n + h\,c_i\,\mathbf{p}_n + h^2 \sum_{j=1}^{s} \alpha_{ij}\,\mathbf{F}(t_n + c_j h, \mathbf{q}^{(j)})\ , \quad i = 1,\ldots,s\ . \tag{4.20}$$

The quantity h is the stepsize of the method which, upon a suitable choice of the parameters $(c_i, a_{ij}, \beta_j, B_j)$, 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 $\mathbf{q}(t)$. Assuming non-vanishing weights B_j we replace the parameters $(c_i, \alpha_{ij}, \beta_j, B_j)$ by new parameters $(\tilde{c}_i, \sigma_{ij}, \hat{c}_j, B_j)$:

$$c_i = \frac{1}{2} + \tilde{c}_i\ , \quad \alpha_{ij} = \left(\sigma_{ij} + \frac{\tilde{c}_i - \hat{c}_j}{2} + \frac{1}{4}\right) B_j\ , \quad \beta_j = \left(\frac{1}{2} - \hat{c}_j\right) B_j \tag{4.21}$$

with $i, j = 1,\ldots,s$. This parametrization turns some useful properties of RKN schemes such as symplecticity and self-adjointness into a set of easily implementable *linear* constraints on the new parameters. Further, some of the order conditions become *homogeneous* equations.

4.1 RKN methods as pRK methods

As observed in [14] a RKN method corresponds to a pRK method applied to the autonomized dynamical system

$$\frac{d}{dt}\begin{pmatrix} t \\ \mathbf{q} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} 1 \\ \mathbf{p} \\ \mathbf{F}(t,\mathbf{q}) \end{pmatrix}$$

equivalent to (4.18). Indeed, the pRK step (3.4) with

$$\mathbf{y} = (t,\mathbf{q})\ , \quad \mathbf{Y} = \mathbf{p}\ , \quad \mathbf{f}(\mathbf{y},\mathbf{Y}) = \mathbf{f}(t,\mathbf{q},\mathbf{p}) \equiv \mathbf{p}\ , \quad \mathbf{F}(\mathbf{y},\mathbf{Y}) \equiv \mathbf{F}(t,\mathbf{q})$$

leads to

$$t_{n+1} = t_n + h \sum_{j=1}^{s} b_j \ , \quad \mathbf{q}_{n+1} = \mathbf{q}_n + h \sum_{j=1}^{s} b_j \, \mathbf{p}^{(j)} \ , \quad \mathbf{p}_{n+1} = \mathbf{p}_n + h \sum_{j=1}^{s} B_j \, \mathbf{F}(t^{(j)}, \mathbf{q}^{(j)})$$

with the internal stages

$$t^{(j)} = t_n + h \sum_{j=1}^{s} a_{ij} \ , \quad \mathbf{q}^{(i)} = \mathbf{q}_n + h \sum_{j=1}^{s} a_{ij} \, \mathbf{p}^{(j)} \ , \quad \mathbf{p}^{(i)} = \mathbf{p}_n + h \sum_{j=1}^{s} A_{ij} \, \mathbf{F}(t^{(j)}, \mathbf{q}^{(j)})$$

with $i = 1, \ldots, s$. Elimination of the internal stages $\mathbf{p}^{(i)}$ in conjunction with the consistency assumption $\sum_j b_j = 1$ yields the RKN step (4.19)/(4.20) with [20, Section 3.5]

$$c_i = \sum_{j=1}^{s} a_{ij} \ , \quad \alpha_{ij} = \sum_{k=1}^{s} a_{ik} \, A_{kj} \ , \quad \beta_j = \sum_{i=1}^{s} b_i \, A_{ij} \ , \quad i, j = 1, \ldots, s \ . \tag{4.22}$$

In terms of the new pRK parameters $(s_{ij}, b_j, S_{ij}, B_j)$ introduced by (3.6) the new RKN parameters $(\tilde{c}_i, \sigma_{ij}, \hat{c}_j, B_j)$ introduced by (4.21) are given by

$$\tilde{c}_i = \sum_{k=1}^{s} s_{ik} \, b_k \ , \quad \sigma_{ij} = \sum_{k=1}^{s} s_{ik} \, b_k \, S_{kj} \ , \quad \hat{c}_j = -\sum_{k=1}^{s} b_k \, S_{ik} \ , \quad i, j = 1, \ldots, s \ . \tag{4.23}$$

4.2 Self-adjoint RKN methods

The adjoint map $\Psi_h^* := (\Psi_{-h})^{-1}$ of the RKN scheme with parameters $(c_i, \alpha_{ij}, \beta_j, B_j)$ is given by the RKN scheme with parameters $(c_i^*, \alpha_{ij}^*, \beta_j^*, B_j^*)$:

$$c_i^* = 1 - c_i \ , \ \alpha_{ij}^* = \alpha_{ij} + B_j - \beta_j - c_i \, B_j \ , \ \beta_j^* = B_j - \beta_j \ , \ B_j^* = B_j \tag{4.24}$$

with $i, j = 1, \ldots, s$. Self-adjoint methods are given by parameters satisfying the symmetry

$$c_{\pi(i)} = 1 - c_i \ , \ \alpha_{\pi(i)\pi(j)} = \alpha_{ij} + B_j - \beta_j - c_i \, B_j \ , \ \beta_{\pi(j)} = B_j - \beta_j \ , \ B_{\pi(j)} = B_j$$

with $i, j = 1, \ldots, s$ and some permutation $\pi : \{1, \ldots, s\} \mapsto \{1, \ldots, s\}$. This is a simple consequence of (4.24) in conjunction with the fact that any permutation of the parameters only permutes the internal stages $\mathbf{q}^{(i)}$ in (4.20) without changing the mapping Ψ_h. In terms of the new parameters $(\tilde{c}_i, \sigma_{ij}, \hat{c}_j, B_j)$ self-adjointness amounts to

$$\tilde{c}_{\pi(i)} = -\tilde{c}_i \ , \ \sigma_{\pi(i)\pi(j)} = \sigma_{ij} \ , \ \hat{c}_{\pi(i)} = -\hat{c}_i \ , \ B_{\pi(j)} = B_j \ , \ i, j = 1, \ldots, s \tag{4.25}$$

with an arbitrary permutation π.

4.3 Symplectic RKN methods

Suris [23] showed (see also [6]) that the RKN method (4.19)/(4.20) is symplectic when applied to a Hamiltonian system $d^2\,\mathbf{q}/dt^2 = -\nabla_{\mathbf{q}} V(\mathbf{q}, t)$, if

$$\beta_j = B_j(1 - c_j)\ , \quad B_i\,\alpha_{ij} - B_j\,\alpha_{ji} = B_i\,B_j\,(c_i - c_j)\ , \quad i, j = 1, \ldots, s\ . \tag{4.26}$$

For irreducible methods, a proof of necessity, is given in [3]. In terms of the new parameters $(\tilde{c}_i, \sigma_{ij}, \hat{c}_j, B_j)$ symplecticity simplifies, without loss of generality for irreducible methods, to the *linear* constraints

$$\hat{c}_j = \tilde{c}_j\ , \quad \sigma_{ij} = \sigma_{ji}\ , \quad i, j = 1, \ldots, s\ . \tag{4.27}$$

4.4 Order theory

Following Hairer et al. [10] the conditions on the RKN parameters to define a method of some specific order may be formulated via **special Nyström rooted trees** (sNr-trees) $\sigma\nu\rho\tau = [(V, E, r, \text{colour})]$. They are bi-colour rooted trees with the additional properties

- children have a different colour than their parents,
- a white vertex has at most one child.

We note that, in contrast to [6], [7], [10], [20], we do not insist on black roots. Vertices without children shall be called **terminal**. For an sNr-tree $\sigma\nu\rho\tau = [(V, E, r, \text{colour})]$ we introduce the notation

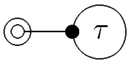
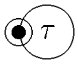
$$\begin{aligned} B = \{\, j \in V\ ;\ \text{colour}(j) = \text{black} \,\}\ , \quad W = \{\, j \in V\ ;\ \text{colour}(j) = \text{white} \,\}\ , \\ BW = \{\, (i, j) \in E\ ;\ i \in B\ ,\ j \in W\ ,\ j \text{ is terminal} \,\}\ , \\ BWB = \{\, (i, j, k) \in V \times V \times V\ ;\ (i, j) \in E\ ,\ (j, k) \in E\ ,\ i, k \in B\ ,\ j \in W \}\ . \end{aligned} \tag{4.28}$$

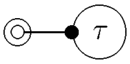
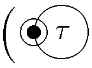
The subset BW of E consists of all edges $\bullet\!\!-\!\!\!-\!\!\circ$ with a white leaf, BWB represents the "double edges" $\bullet\!\!-\!\!\!-\!\!\circ\!\!-\!\!\!-\!\!\bullet$ consisting of black grandparents/grandchildren with a white parent in between. Following [10] we define the RKN weights of a method $(c_i, \alpha_{ij}, \beta_j, B_j)$ by

$$\Phi_{RKN}(\sigma\nu\rho\tau) \;=\; \sum_{n_1=1}^{s} \cdots \sum_{n_{|B|}=1}^{s} B_{n_r} \Big(\prod_{(i,j,k)\in BWB} \alpha_{n_i n_k} \Big) \Big(\prod_{(i,j)\in BW} c_{n_i} \Big) \tag{4.29}$$

and

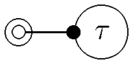
$$\Psi_{RKN}(\sigma\nu\rho\tau) \;=\; \sum_{n_1=1}^{s} \cdots \sum_{n_{|B|}=1}^{s} \beta_{n_r} \Big(\prod_{(i,j,k)\in BWB} \alpha_{n_i n_k} \Big) \Big(\prod_{(i,j)\in BW} c_{n_i} \Big) \tag{4.30}$$

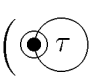
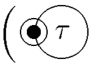
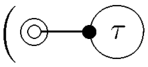
for trees with a black root $r \in V$. The products are to be understood as 1, if either BWB or BW is empty, $|B|$ denotes the number of black vertices. It is convenient to interpret the polynomials Ψ_{RKN} as weights associated with trees with white roots. They have the form  with some special Nyström sub-tree τ. Shifting the root to the adjacent black vertex and chopping off the original white root one obtains the sNr-tree . We define

$\Phi_{RKN}\Big($  $\Big) \;:=\; \Psi_{RKN}\Big($  $\Big)$

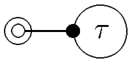
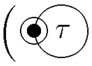
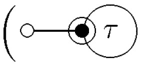
as the RKN weight of trees with a white root, supplemented by $\Phi_{RKN}(◎) := 1$ for an isolated white root. The order conditions of a RKN method are given by

[10, Theorem 13.12]: *The RKN method (4.19)/(4.20) is of order N if and only if its parameters satisfy $\Phi_{RKN}(\sigma\nu\rho\tau) = 1/\gamma(\sigma\nu\rho\tau)$ for all sNr-trees $\sigma\nu\rho\tau$ through N vertices.*

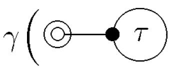
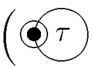
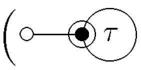
We note that the order conditions associated with trees  with white roots and arbitrary special Nyström sub-trees τ with $|\tau|$ vertices represent the equations

$\Psi_{RKN}\Big($  $\Big) \;=\; \dfrac{1}{(1+|\tau|)\,\gamma\Big(}$  $\Big) \;=\; \dfrac{1}{\gamma\Big(}$  $\Big)$

involving trees with black roots through $N-1$ vertices. The first of the symplecticity conditions (4.26), $\beta_j = B_j(1-c_j)$, serves as a simplifying assumption. From the definition of the RKN weight one immediately finds the relation:

$\Phi_{RKN}\Big($  $\Big) \;=\; \Phi_{RKN}\Big($  $\Big) \;-\; \Phi_{RKN}\Big($  $\Big)$

with arbitrary special Nyström sub-trees τ. Observing

$\dfrac{1}{\gamma\Big(}$  $\Big) \;=\; \dfrac{1}{\gamma\Big(}$  $\Big) \;-\; \dfrac{1}{\gamma\Big(}$  $\Big)$

the order equations $\Phi_{RKN}(\sigma\nu\rho\tau) - 1/\gamma(\sigma\nu\rho\tau) = 0$ associated with trees with white roots are linear combinations of those associated with trees with black roots. Only sNr-trees with black roots need to be considered [10, Lemma 13.13].

4.5 Modified order conditions

Using the new parameters $(\tilde{c}_i, \sigma_{ij}, \hat{c}_j, B_j)$ introduced by (4.21) we define the following modified RKN weight:

Definition 4.1 *Using the notation (4.28) the* **modified RKN weight** *for an sNr-tree $\sigma\nu\rho\tau = [(V, E, r, \mathrm{colour})]$ with $|B|$ black vertices is defined by*

$$\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) \;=\; \sum_{n_1=1}^{s} \cdots \sum_{n_{|B|}=1}^{s} \Big(\prod_{i\in B} B_{n_i}\Big)\Big(\prod_{(i,j,k)\in BWB} \sigma_{n_i n_k}\Big)\Big(\prod_{(i,j)\in BW} \tilde{c}_{n_i}\Big)\;,$$

if the root is black. We define

$$\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) \;=\; -\sum_{n_1=1}^{s}\cdots\sum_{n_{|B|}=1}^{s} \hat{c}_{n_{r'}}\Big(\prod_{i\in B} B_{n_i}\Big)\Big(\prod_{(i,j,k)\in BWB} \sigma_{n_i n_k}\Big)\Big(\prod_{(i,j)\in BW} \tilde{c}_{n_i}\Big)$$

for sNr-trees $\sigma\nu\rho\tau = [(V, E, r, \text{colour})] = \circledcirc\!\!-\!\!\bullet\,\tau$ *with a white root and an arbitrary special Nyström sub-tree* τ*. Here* r' *is the label of the black vertex adjacent to the white root, i.e.,* r' *labels the black root of the associated tree* $\bullet\,\tau$*. For an isolated white root we put* $\tilde{\Phi}_{RKN}(\circledcirc) := 1$*.*

Pictorially, $\tilde{\Phi}_{RKN}$ is obtained by attaching a copy of the vector (B_j) to any black vertex, a copy of the matrix (σ_{ij}) to any "double edge" $\bullet\!-\!\circ\!-\!\bullet$ in BWB and a copy of the vector $(\tilde{c}_i)$ to the terminal edges $\bullet\!-\!\circ$ in BW. In case of a white root, the vector $(-\hat{c}_j)$ is attached to the edge emerging from the white root.

The modified weights are obtained by replacing

$$c_i \mapsto \tilde{c}_i \;, \quad a_{ij} \mapsto \sigma_{ij}\, B_j \;, \quad \beta_j \mapsto -\hat{c}_j\, B_j \;, \quad i, j = 1, \ldots, s$$

in the definition of Φ_{RKN}. One obtains the analogue of lemma 3.2:

Lemma 4.2 *For any sNr-tree* $\sigma\nu\rho\tau$ *with* $|E|$ *edges:*

$$\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) \;=\; \Phi_{RKN}(\sigma\nu\rho\tau) \;+\; \sum_{k=1}^{|E|}\left(-\frac{1}{2}\right)^k \sum_{C_k(\sigma\nu\rho\tau)} \Phi_{RKN}(\sigma\nu\rho\tau_0)\cdots\Phi_{RKN}(\sigma\nu\rho\tau_k) \;,$$

where C_k *denotes the set of all* $\binom{|E|}{k}$ *k-partitions, each inducing a decomposition of* $\sigma\nu\rho\tau$ *into the sNr-sub-trees* $\sigma\nu\rho\tau_0, \ldots, \sigma\nu\rho\tau_k$*.*

Proof Following subsection 4.1 we construct a pRK scheme $(a_{ij}, b_j, A_{ij}, B_j)$ which is equivalent to the RKN scheme $(c_i, \alpha_{ij}, \beta_j, B_j)$ via (4.22). Choose any invertible matrix (a_{ij}) satisfying the row-sum conditions $c_i = \sum_j a_{ij}$. Inverting (a_{ij}) one constructs $(A_{ij}) = (a_{ij})^{-1}(\alpha_{ij})$. If (α_{ij}) is invertible, then so is (A_{ij}) and one obtains the weights $(b_j) = (\beta_j)(A_{ij})^{-1}$. Comparing the definitions (3.11)/(3.12) of the pRK weights with the definitions (4.29)/(4.30) of the RKN weights one sees that (4.22) implies $\Phi_{pRK}(\sigma\nu\rho\tau) = \Phi_{RKN}(\sigma\nu\rho\tau)$ for arbitrary sNr-trees. Introducing (s_{ij}, S_{ij}) according to (3.6) one obtains the parameters $(\tilde{c}_i, \sigma_{ij}, \hat{c}_j, B_j)$ of (4.21) via (4.23). Comparing the definitions 3.1 and 4.1 one sees that (4.23) implies $\tilde{\Phi}_{pRK}(\sigma\nu\rho\tau) = \tilde{\Phi}_{RKN}(\sigma\nu\rho\tau)$ for arbitrary sNr-trees. Thus lemma 3.2 leads to the desired result which extends to degenerate matrices (α_{ij}) via continuity. □

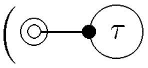
Since both $\tilde{\Phi}_{RKN}$ and $\tilde{\delta}$ are obtained from Φ_{RKN} and $1/\gamma$ by the same deformation process, one has the analogue of (3.14) and induction on the number of vertices immediately leads to:

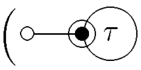
Theorem 4.3 *The order conditions $\Phi_{RKN}(\sigma\nu\rho\tau) = 1/\gamma(\sigma\nu\rho\tau)$ for an RKN scheme are satisfied for all sNr-trees $\sigma\nu\rho\tau$ through N vertices if and only if $\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) = \tilde{\delta}(\sigma\nu\rho\tau)$ holds for all sNr-trees through N vertices.*

Symplecticity serves as a simplifying assumption for RKN schemes [6]:

Theorem 4.4 *For symplectic RKN schemes the new order conditions $\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) = \tilde{\delta}(\sigma\nu\rho\tau)$ are invariant under root-shifting. The scheme is of order N if and only if these order conditions are satisfied for one rooted sNr-representative $\sigma\nu\rho\tau$ for every non-rooted special Nyström tree through N vertices.*

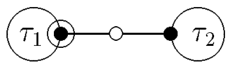
Proof The first condition $\hat{c}_j = \tilde{c}_j$ in (4.27) immediately leads to the relation

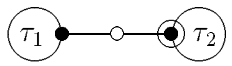
$\tilde{\Phi}_{RKN}\Big($ 

$\Big) = -\,\tilde{\Phi}_{RKN}\Big($ 

$\Big)$

for all sNr-trees with a white root and an arbitrary special Nyström sub-tree τ. The symmetry of the matrix (σ_{ij}) yields

$\tilde{\Phi}_{RKN}\Big($ 

$\Big) = \tilde{\Phi}_{RKN}\Big($ 

$\Big)$

for all trees of the indicated form with arbitrary special Nyström sub-trees τ_1, τ_2: root-shifting along a double edge $(i,j,k) \in BWB$ only leads to a replacement $\sigma_{n_i n_k} \mapsto \sigma_{n_k n_i}$ in the definition of $\tilde{\Phi}$ (in the root-shifted tree the new double edge is (k,j,i)). With the root-shifting property of $\tilde{\delta}$ as stated in lemma 2.3.i) the new order equations $\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) = \tilde{\delta}(\sigma\nu\rho\tau)$ are independent of the location of the root, if the RKN scheme is symplectic. □

For self-adjoint RKN schemes one finds the analogue of theorem 3.5:

Theorem 4.5 *For self-adjoint RKN schemes the new order conditions $\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) = \tilde{\delta}(\sigma\nu\rho\tau)$ are automatically satisfied for all sNr-trees $\sigma\nu\rho\tau$ with an even number of vertices.*

Proof The symmetry (4.25) of self-adjoint schemes immediately leads to $\tilde{\Phi}_{RKN}(\sigma\nu\rho\tau) = 0$ for all special Nyström rooted trees with an even number of vertices: there is an odd number of edges introducing minus signs $\hat{c}_{\pi(i)} = -\hat{c}_i$, $\tilde{c}_{\pi(i)} = -\tilde{c}_i$ after re-summation $n_i \mapsto \pi(n_i)$, $i = 1, \ldots, |B|$, in definition 4.1. Further, with lemma 2.3.ii) $\tilde{\delta}(\sigma\nu\rho\tau) = 0$ for even trees, whence the new order equations are automatically satisfied. □

Remark 4.6 *In the new order framework the attributes of symplecticity (4.27) and self-adjointness (4.25) are easily implemented. With $\pi(i) = s+1-i$ any RKN method with parameters*

$$(\tilde{c}_i) = (\hat{c}_i) = (\tilde{c}_1, \tilde{c}_2, \ldots, -\tilde{c}_2, -\tilde{c}_1)\ , \quad (B_j) = (B_1, B_2, \ldots, B_2, B_1) \tag{4.31}$$

and

$$
(\sigma_{ij}) = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \dots & \dots & \sigma_{1s} \\ \sigma_{12} & \sigma_{22} & \iddots & \iddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \sigma_{22} & \sigma_{12} \\ \sigma_{1s} & \dots & \iddots & \sigma_{12} & \sigma_{11} \end{pmatrix} \tag{4.32}
$$

is both self-adjoint and symplectic. Explicit symplectic methods are obtained by

$$
\sigma_{ij} \;=\; \sigma_{ji} \;=\; \frac{\tilde{c}_j - \tilde{c}_i}{2} \;-\; \frac{1}{4}\,, \quad 1 \le i \le j \le s\ . \tag{4.33}
$$

In conjunction with (4.31) these schemes are self-adjoint.

The number of free parameters for a general s-stage RKN method is $s(s+3)$. For a symplectic method under the new parametrization (4.21) this reduces to $s(s+5)/2$ free parameters taking into account (4.27). For the most general symplectic self-adjoint RKN method (4.31)/(4.32) the number of free parameters is $\lfloor (s+1)^2/4 \rfloor + s$. An explicit symplectic RKN method (4.33) is prescribed by $2\,s$ free parameters $\tilde{c}_1, \dots, \tilde{c}_s$, $B_1, \dots, B_s$. With the (4.31) the most general explicit self-adjoint RKN method is prescribed by s parameters. Note that, for even s, the latter two quantities are identical to the partitioned case in section 3.4. However, there are less order equations to be solved in the explicit Nyström case and hence higher order is generally attainable [5].

5 Conclusions

We have outlined a modification of standard Butcher theory applicable to partitioned and Runge-Kutta-Nyström methods. Our new weight function has the advantage that it encrypts desirable properties such as symplecticity and self-adjoincy in a natural manner, solely by imposing simple symmetries among the parameters.

In Butcher's formalism the density of a tree can be computed via a simple recursion. In the new formalism, derivation of the (reciprocal of) density becomes a more involved process. However, this is of marginal importance. The definition of the new densities for an important class of trees was derived using generating functions in [22]. Furthermore, since the partitioning process is defined algorithmically it becomes possible to implement the derivation in a computer algebra system [13, 22].

The advantages of this approach include a reduction in the parameter space, coupled with the fact that lower order dependencies are filtered out of the weight function. This should be of considerable benefit when solving the order constraints analytically using an automated approach such as Gröbner bases [8, 21]. We have already used such a technique to good effect in a complete classification of self-adjoint symplectic Runge-Kutta methods through $s = 6$ stages [13].

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?? [25] Turchetti has a nice example (from plasma physics???) but I can't find the reference right now...

Appendix

We consider the deformation

$$a_{ij}^{(\epsilon)} = a_{ij} + \epsilon\, b_j \ , \quad A_{ij}^{(\epsilon)} = A_{ij} + \epsilon\, B_j \ , \quad \epsilon \in \mathbb{R}$$

of the pRK parameters. Replacing $(a_{ij}), (A_{ij})$ by these deformed quantities in (3.11) and (3.12) we define deformed pRK weights $\Phi_{pRK}^{(\epsilon)}(\beta\rho\tau)$. We show

$$\Phi_{pRK}^{(\epsilon)}(\beta\rho\tau) = \Phi_{pRK}(\beta\rho\tau) + \sum_{k=1}^{|E|} \epsilon^k \sum_{C_k(\beta\rho\tau)} \Phi_{pRK}(\beta\rho\tau_0)\Phi_{pRK}(\beta\rho\tau_1)\cdots\Phi_{pRK}(\beta\rho\tau_k) \ . \tag{A.1}$$

For $\epsilon = -1/2$ one finds

$$a_{ij}^{(-1/2)} = a_{ij} - \frac{b_j}{2} = s_{ij}\, b_j \ , \quad A_{ij}^{(-1/2)} = A_{ij} - \frac{B_j}{2} = S_{ij}\, B_j \ ,$$

i.e., $\Phi_{pRK}^{(-1/2)} = \tilde{\Phi}_{pRK}$, whence (A.1) leads to lemma 3.2. For a formal proof of (A.1) we deform the copies of the matrices (a_{ij}) and (A_{ij}) only on a subset $D \subset E$ of the edges and inductively increase the cardinality $|D|$ from 0 to $|E|$. We define

$$\Phi_{pRK}^{(\epsilon)}(\beta\rho\tau, D) \ = $$
$$\sum_{n_1=1}^{s} \cdots \sum_{n_{|V|}=1}^{s} \beta_{n_r} \Big(\prod_{\substack{(i,k)\in D \\ k\in W}} a_{n_i n_k}^{(\epsilon)} \Big) \Big(\prod_{\substack{(i,k)\in E\setminus D \\ k\in W}} a_{n_i n_k} \Big) \Big(\prod_{\substack{(i,k)\in D \\ k\in B}} A_{n_i n_k}^{(\epsilon)} \Big) \Big(\prod_{\substack{(i,k)\in E\setminus D \\ k\in B}} A_{n_i n_k} \Big)$$

for a tree $\beta\rho\tau = [(V, E, r, \text{colour})]$ with $|V| = |E| + 1$ vertices. Here $\beta_j = B_j$, if the root is black, and $\beta_j = b_j$, if the root is white. For $\epsilon = 0$ or $D = \emptyset$ this is the standard pRK weight, for $\epsilon = -1/2, D = E$ one obtains the modified pRK weight of definition 3.1. The set of all k-partitionings involving edges in D shall be denoted by

$$C_k(\beta\rho\tau, D) := \{\ \{e_1, \ldots, e_k\}\ ;\ e_1, \ldots, e_k \in D \text{ mutually distinct }\}\ ,$$

the set of all $(k+1)$-partitionings involving k edges in D and a given edge $e \notin D$ shall be denoted by

$$C_{k+1}^{e}(\beta\rho\tau, D) = \{\ \{e\} \cup c\ ;\ c \in C_k(\beta\rho\tau, D)\ \}\ .$$

The following lemma yields (A.1) for $D = E$:

Lemma A.1 *For any $D \subset E$:*

$$\Phi_{pRK}^{(\epsilon)}(\beta\rho\tau, D) = \sum_{k=0}^{|D|} \epsilon^k \sum_{C_k(\beta\rho\tau, D)} \Phi_{pRK}(\beta\rho\tau_0)\Phi_{pRK}(\beta\rho\tau_1) \cdots \Phi_{pRK}(\beta\rho\tau_k)\ .$$

Proof For $|D| = 0$ the statement is obvious. For the inductive step $|D| \mapsto |D| + 1$ with $|D| < |E|$ one chooses an arbitrary edge $e \in E \setminus D$ and considers the two trees $\beta\rho\tau_I$, $\beta\rho\tau_{II}$ obtained by chopping e from $\beta\rho\tau$. From the definition of the deformed pRKN weight one immediately finds

$$\Phi_{pRK}^{(\epsilon)}(\beta\rho\tau, D \cup \{e\}) = \Phi_{pRK}^{(\epsilon)}(\beta\rho\tau, D) + \epsilon\, \Phi_{pRK}^{(\epsilon)}(\beta\rho\tau_I, E_I \cap D)\ \Phi_{pRK}^{(\epsilon)}(\beta\rho\tau_{II}, E_{II} \cap D)\,, \tag{A.2}$$

where E_I and E_{II} are the edges of τ_I and τ_{II}, respectively (i.e., $E = \{e\} \cup E_I \cup E_{II}$). Using the inductive assumption one has

$$\Phi_{pRK}^{(\epsilon)}(\beta\rho\tau_I, E_I \cap D) \quad = \quad \sum_{k_I=0}^{|E_I \cap D|} \epsilon^{k_I} \sum_{C_{k_I}(\beta\rho\tau_I, E_I \cap D)} \Phi_{pRK}(\beta\rho\tau_{I0}) \cdots \Phi_{pRK}(\beta\rho\tau_{Ik_I})\ ,$$

$$\Phi_{pRK}^{(\epsilon)}(\beta\rho\tau_{II}, E_{II} \cap D) \quad = \quad \sum_{k_{II}=0}^{|E_{II} \cap D|} \epsilon^{k_{II}} \sum_{C_{k_{II}}(\beta\rho\tau_{II}, E_{II} \cap D)} \Phi_{pRK}(\beta\rho\tau_{II0}) \cdots \Phi_{pRK}(\beta\rho\tau_{IIk_{II}})\ ,$$

whence

$$\Phi^{(\epsilon)}_{pRK}(\beta\rho\tau_I, E_I \cap D)\ \Phi^{(\epsilon)}_{pRK}(\beta\rho\tau_{II}, E_{II} \cap D) =$$
$$\sum_{k=0}^{|D|} \epsilon^k \sum_{\substack{k_I, k_{II} \\ k_I + k_{II} = k}} \sum_{\substack{C_{k_I}(\beta\rho\tau_I, E_I \cap D), \\ C_{k_{II}}(\beta\rho\tau_{II}, E_{II} \cap D)}} \Phi_{pRK}(\beta\rho\tau_{I0}) \cdots \Phi_{pRK}(\beta\rho\tau_{Ik_I}) \times \Phi_{pRK}(\beta\rho\tau_{II0}) \cdots \Phi_{pRK}(\beta\rho\tau_{IIk_{II}}) \ .$$

The sub-trees $\beta\rho\tau_{I0}, \ldots, \beta\rho\tau_{IIk_{II}}$ arise by chopping $k_I + k_{II}$ edges in D together with e from $\beta\rho\tau$, whence the right hand side may be written as

$$\sum_{k=0}^{|D|} \epsilon^k \sum_{C^e_{k+1}(\beta\rho\tau, D)} \Phi_{pRK}(\beta\rho\tau_0) \cdots \Phi_{pRK}(\beta\rho\tau_{k+1}) \ .$$

Insertion into (A.2) together with the inductive assumption for $\Phi^{(\epsilon)}_{pRK}(\beta\rho\tau, D)$ leads to

$$\begin{aligned} \Phi^{(\epsilon)}_{pRK}(\beta\rho\tau, D \cup \{e\}) \ = \ & \sum_{k=0}^{|D|} \epsilon^k \sum_{C_k(\beta\rho\tau, D)} \Phi_{pRK}(\beta\rho\tau_0) \cdots \Phi_{pRK}(\beta\rho\tau_k) \\ & + \sum_{k=0}^{|D|} \epsilon^{k+1} \sum_{C^e_{k+1}(\beta\rho\tau, D)} \Phi_{pRK}(\beta\rho\tau_0) \cdots \Phi_{pRK}(\beta\rho\tau_{k+1}) \ . \end{aligned}$$

With

$$\sum_{C_0(\beta\rho\tau, D)} \Phi_{pRK}(\beta\rho\tau_0) \ = \sum_{C_0(\beta\rho\tau, D\cup\{e\})} \Phi_{pRK}(\beta\rho\tau_0) \ = \ \Phi_{pRK}(\beta\rho\tau) \ ,$$
$$\sum_{C_{k+1}(\beta\rho\tau, D)} + \sum_{C^e_{k+1}(\beta\rho\tau, D)} = \sum_{C_{k+1}(\beta\rho\tau, D\cup\{e\})} , \quad k = 0, \ldots, |D| - 1$$

and $C^e_{|D|+1}(\beta\rho\tau, D) = C_{|D|+1}(\beta\rho\tau, D \cup \{e\}) = \{D \cup \{e\}\}$ the desired result

$$\Phi^{(\epsilon)}_{pRK}(\beta\rho\tau, D \cup \{e\}) = \sum_{k=0}^{|D|+1} \epsilon^k \sum_{C_k(\beta\rho\tau, D\cup\{e\})} \Phi_{pRK}(\beta\rho\tau_0)\Phi_{pRK}(\beta\rho\tau_1) \cdots \Phi_{pRK}(\beta\rho\tau_k)$$

is obtained for the deformation of the weight on the increased set of edges $D \cup \{e\}$. □