SYMPLECTIC RUNGE-KUTTA SCHEMES III: CANONICAL ELEMENTARY DIFFERENTIALS*

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Abstract. It has been shown that numerical methods for Hamiltonian systems may be characterised in terms of so-called canonical elementary differentials. Recent results by the authors demonstrate that the symplecticity condition for Runge-Kutta schemes may be eliminated by suitable parametrisation of the order conditions. These results are used to re-examine the relationship between order conditions for canonical Runge-Kutta methods and canonical elementary differentials.

Key words. Runge-Kutta schemes, trees, order conditions, elementary differentials, Hamiltonian systems, symplectic, canonical, generating functions

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1 Introduction.

B-series, named after John Butcher, provide a powerful tool for the categorisation of numerical methods for solving systems of ordinary differential equations. For example, they have been used to explore the effective order of multi-derivative methods, Rosenbrock methods and compositions of Runge-Kutta methods [5, 4]. Compositions of methods with their adjoints have also been studied in the symplectic case [10, 2, 7].

A B-series represents a numerical method in terms of graph-theoretical concepts [5]. Given a system of ordinary differential equations in $\mathbb{R}^d$

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}) \ , \tag{1.1}$$

one can express the Taylor expansion of the solution in the form

$$\mathbf{y}(t+\Delta t) \ = \ \mathbf{y}(t) \ + \ \sum_{r=1}^{\infty} \frac{(\Delta t)^r}{r!} \sum_{\substack{\rho\tau \\ r(\rho\tau)=r}} \alpha(\rho\tau) \ \mathbf{F}(\rho\tau)(\mathbf{y}(t)) \ ,$$

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where $\mathbf{F}(\rho\tau)(\mathbf{y})$ is the *elementary differential* associated with the rooted tree $\rho\tau$. It represents a polynomial expression of the vector field $\mathbf{f}$ and its derivatives obtained by recursively inserting (1.1) into the higher time derivatives of the solution. The coefficient $\alpha(\rho\tau)$ is the number of monotonic labelings of the rooted tree, $r(\rho\tau)$ represents the order of the tree, i.e. the number of vertices. A numerical single-step method for solving (1.1) consists of a mapping

$$\mathbf{y} \quad \mapsto \quad \mathbf{y}^* \;=\; \mathbf{y} \;+\; \sum_{r=1}^{\infty} \frac{h^r}{r!} \sum_{\substack{\rho\tau \\ r(\rho\tau)=r}} c(\rho\tau)\; \mathbf{F}(\rho\tau)(\mathbf{y}) \tag{1.2}$$

where h is the stepsize and the coefficients $c(\rho\tau)$ characterise the specific method. The expression (1.2) is called a *B-series* [5]. For a method of order p the coefficients $c(\rho\tau)$ have to coincide with $\alpha(\rho\tau)$ for all trees of order $r(\rho\tau) \leq p$, so that the B-series approximates the Taylor expansion up to terms $O(h^{p+1})$. The required constraints

$$c(\rho\tau) \;=\; \alpha(\rho\tau) \tag{1.3}$$

are the *order conditions* of the method associated with the rooted trees $\rho\tau$.

A systematic approach for the investigation of the order of symplectic Runge-Kutta methods is provided in [8]. Two equivalent formulations of the order conditions were derived. One, the "homogeneous form", involves a sum over all rootings of a given tree. It is equivalent to the order condition for a single rooted representative of that tree. In [11] the order conditions are re-derived in terms of modified weights and densities which satify the symplecticity constraints identically and further resolve the distinction between the two formulations. The new order conditions are invariant under root-shifting, i.e. they coincide for different rootings of a tree. The main result is that for Runge-Kutta methods only one order condition per non-rooted (non-superfluous) tree arises. In [3] it is shown that this result holds for arbitrary symplectic B-series, not necessarily of Runge-Kutta type.

As canonical transformations, symplectic B-series are associated with suitable generating functions. For Runge-Kutta schemes the order conditions arise from Taylor expansion with respect to the stepsize of a scalar function, Γ, derived from the generating function. This approach leads to the concept of canonical elementary differentials. In [8] it was shown that Γ involves the homogeneous form of the order conditions, i.e. it involves a sum over different rooted trees.

We show that with the new order conditions, the expansion of Γ can be formulated in terms of only one rooted representative per tree. A similar argument applies to the derivation of methods which minimise the principal error function [12].

2 Graph theoretical definitions.

We briefly summarise the graph theoretical notions necessary for the discussion of order-conditions for symplectic Runge-Kutta schemes.

i. A *labeled tree*, $\lambda\tau$, of *order* $r(\lambda\tau) = r$ consists of the set of vertices $V = \{1, \cdots, r\}$ and a set E of unordered pairs (edges) $\{v, w\}$ of vertices $v, w \in V$, $v \neq w$.

ii. Two labeled trees are *isomorphic* if there is a one-to-one correspondence between vertices which preserves adjacency. A *tree*, τ, is thus an equivalence class comprising a labeled tree and all labeled trees isomorphic to it. An *automorphism* of a labeled tree is an isomorphism to itself.

iii. The number of all automorphisms of a labeled tree $\lambda\tau \in \tau$ is independent of the labeling. The *symmetry* $\sigma(\tau)$ of a tree is the number of automorphisms of any labeled representative.

iv. A *rooted labeled tree* $\rho\lambda\tau = (V, E, \rho)$ is a labeled tree where a special vertex $\rho \in V$ (the root) is highlighted. The edges can be regarded as ordered pairs (f, s) reflecting their father/son relationship induced by the root. A *rooted tree* $\rho\tau$ is the equivalence class modulo isomorphisms preserving the root. The *symmetry* $\sigma(\rho\tau)$ is the number of all automorphisms preserving the root.

v. In a *monotonically labeled rooted tree* $f < s$ for all father/son pairs $(f, s) \in E$. For a rooted tree $\rho\tau$ we denote by $\alpha(\rho\tau)$ the *number of its monotonically labeled rooted trees.*

vi. The *density*, $\gamma(\rho\tau)$, of a rooted tree is a measure of its "bushiness". It may be defined recursively [1] (see also [11]) and satisfies

$$\alpha(\rho\tau)\;\gamma(\rho\tau)\;\sigma(\rho\tau) \;=\; r(\rho\tau)!\;.$$

vii. Let $\beta(\rho\tau)$ denote the *number of ways of labeling a rooted tree with* $r(\rho\tau)-1$ *distinct labels* on condition that the root is not labeled, but every other vertex is labeled. It satisfies [1]

$$r(\rho\tau)\;\beta(\rho\tau) \;=\; \alpha(\rho\tau)\;\gamma(\rho\tau)\;.$$

viii. Let $\bar{\beta}(\rho\tau)$ denote the *number of ways of labeling a rooted tree with* $r(\rho\tau)$ *distinct labels* so that every vertex is labeled:

$$\bar{\beta}(\rho\tau) \;=\; r(\rho\tau)\;\beta(\rho\tau) \;=\; \alpha(\rho\tau)\;\gamma(\rho\tau)\;.$$

ix. The *similarity*, $\varsigma(\rho\tau)$, of a rooted tree $\rho\tau = (V, E, \rho) \in \tau$ is the number of ways of rooting the tree τ to obtain the rooted tree $\rho\tau$. Formally:

$$R(\rho\tau) \;=\; \Big\{\; \rho' \in V\;;\; (V, E, \rho') \text{ is isomorphic to } (V, E, \rho) \;\Big\}\;,$$

and $\varsigma(\rho\tau) = |R(\rho\tau)|$, the number of elements in $R(\rho\tau)$.

x. Let $\rho\tau_1$ and $\rho\tau_2$ be two rooted trees belonging to the same tree τ, differing only in the location of the root. These trees are of the same (respectively different) *parity* if the length of the path between the roots is an even (respectively odd) integer.

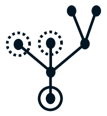

Figure 1: A rooted tree with $\varsigma(\rho\tau) = 3$.

Apart from ix. these notions and their relevance in the context of numerical methods are well-established [1]. Here we illustrate the concept of similarity:

Example 2.1 The rooted tree given in figure 1 has $\varsigma(\rho\tau) = 3$, since there are two alternative roots, indicated by dashed circles, which give rise to the same rooted tree.

A *superfluous* tree consists of two copies of a tree joined by an edge [8, 11]. In a *centroid* of a tree the root is chosen such that the longest path is minimised. As there are at most two centroids for each tree one has

Example 2.2 All centroids of non-superfluous trees have $\varsigma(\rho\tau) = 1$.

The notion of similarity provides a connection between the symmetry of rooted and unrooted trees:

Lemma 2.1 *For any $\rho\tau \in \tau$:* $\quad \sigma(\tau) \; = \; \varsigma(\rho\tau)\; \sigma(\rho\tau)$.

Proof For any $\rho' \in R(\rho\tau)$ fix an isomorphism $j_{\rho'} : \; (V, E, \rho) \mapsto (V, E, \rho')$.
i) Let i' be an automorphism of $\rho\tau$. Then $k := j_{\rho'} \circ i'$ is an automorphism of τ. There are $\varsigma(\rho\tau)$ choices for ρ' and $\sigma(\rho\tau)$ choices for i'. Each choice yields a different automorphism k of τ, since $j_{\rho'} \circ i' = j_{\rho''} \circ i''$ implies $\rho' = \rho''$ and $i' = i''$. Therefore there exist at least $\varsigma(\rho\tau)\sigma(\rho\tau)$ different automorphisms of τ and we have: $\varsigma(\rho\tau)\sigma(\rho\tau) \le \sigma(\tau)$.
ii) Let k be an automorphism of τ. Define $\rho' := k(\rho)$ and consider the automorphism $i' = j_{\rho'}^{-1} \circ k$. Hence for each k there exists *uniquely* an element $\rho' \in R(\rho\tau)$ and an automorphism i' of $\rho\tau$ such that $k = j_{\rho'} \circ i'$. Since there are at most $\varsigma(\rho\tau)$ distinct ρ' and at most $\sigma(\rho\tau)$ distinct i', arising from all possible choices of k, we have: $\sigma(\tau) \le \varsigma(\rho\tau)\sigma(\rho\tau)$.
□

3 Review of canonical elementary differentials.

An approach for the investigation of order of one-step symplectic numerical methods (not necessarily Runge-Kutta schemes) is provided in [8]. The approach relies on a Taylor series expansion of a suitable generating function. This technique has been used to construct canonical B-series [3]. One result is a proof of the necessity of the symplecticity condition [9] for Runge-Kutta methods. A second result is the proof that no multi-derivative symplectic Runge-Kutta methods exist [6]. We review the application of this theory to Runge-Kutta methods and then we show how the results can be simplified in the light of the framework presented in [11].

Consider a Hamiltonian system

$$\frac{d\mathbf{y}}{dt} = \frac{d}{dt}\begin{pmatrix}\mathbf{q}\\ \mathbf{p}\end{pmatrix} = \mathbf{f}(\mathbf{y}) = \begin{pmatrix}H_{\mathbf{p}}\\ -H_{\mathbf{q}}\end{pmatrix} \tag{3.1}$$

where subscripts represent the derivatives of the Hamiltonian function $H(\mathbf{q},\mathbf{p})$. Assume that the B-series (1.2) is generated by an s-stage Runge-Kutta method

$$\begin{aligned} \mathbf{y}_i &= \mathbf{y} + h\sum_{j=1}^{s} a_{ij}\,\mathbf{f}(\mathbf{y}_j)\ , \qquad i = 1,\ldots,s\ , \\ \mathbf{y}^* &= \mathbf{y} + h\sum_{i=1}^{s} b_i\,\mathbf{f}(\mathbf{y}_i)\ , \end{aligned} \tag{3.2}$$

where b_i and a_{ij} are the parameters of the scheme which have to be determined from the order conditions. The weights of the corresponding B-series are given by [3]

$$c(\rho\tau) = \alpha(\rho\tau)\,\gamma(\rho\tau)\,\Phi(\rho\tau)\ ,$$

where Φ is a polynomial of the parameters [1, 11]. The order conditions (1.3) become

$$\Phi(\rho\tau) = \frac{1}{\gamma(\rho\tau)}\ .$$

If the Runge-Kutta method is symplectic, i.e. [11]

$$a_{ij} = \left(\frac{1}{2} + s_{ij}\right) b_j \tag{3.3}$$

with an arbitrary skew-symmetric matrix (s_{ij}), then a generating function for the Runge-Kutta map $\mathbf{y} = (\mathbf{q},\mathbf{p})^T \mapsto \mathbf{y}^* = (\mathbf{q}^*,\mathbf{p}^*)^T$ is given by

$$S(\mathbf{p},\mathbf{q}^*,h) = <\mathbf{p},\mathbf{q}^*> - h\sum_{i=1}^{s} b_i\,H(\mathbf{y}_i) - h^2\sum_{i,j=1}^{s} b_i\,a_{ij} < H_{\mathbf{p}}(\mathbf{y}_i), H_{\mathbf{q}}(\mathbf{y}_j) >\ ,$$

i.e. the mapping (3.2) is given implicitly by

$$\mathbf{q} = \frac{\partial S}{\partial \mathbf{p}}\ , \quad \mathbf{p}^* = \frac{\partial S}{\partial \mathbf{q}^*}\ . \tag{3.4}$$

This result is attributed to F. Lasagni in [8]. The order conditions arise from derivatives of the generating function with respect to the stepsize. The mapping defined by (3.4) is consistent with (3.1), of order $n \geq 2$ if and only if $\sum_i b_i = 1$ and [8]

$$\left.\frac{\partial^{r-1}\Gamma}{\partial h^{r-1}}\right|_{\mathbf{q},\mathbf{p},h=0} = 0\ , \quad r = 2,\ldots,n\ , \tag{3.5}$$

where

$$\Gamma = \frac{\partial}{\partial h} S(\mathbf{p}, \mathbf{q}^*, h) \ .$$

In (3.5) the derivatives have to be taken with constant values of $\mathbf{q}$ and $\mathbf{p}$, whereas constant $\mathbf{p}$ and $\mathbf{q}^*$ are assumed in the other formulae. For canonical Runge-Kutta methods one finds [8]

$$\Gamma = -\sum_{i=1}^{s} b_i H(\mathbf{y}_i)$$

and Taylor expansion leads to

$$\left.\frac{\partial^{r-1}\Gamma}{\partial h^{r-1}}\right|_{\mathbf{q},\mathbf{p},h=0} = -\frac{1}{r} \sum_{\substack{\rho\tau \\ r(\rho\tau)=r}} \alpha(\rho\tau)\,\gamma(\rho\tau)\,\Phi(\rho\tau)\,\theta(\rho\tau) \ , \qquad r \geq 2 \ . \tag{3.6}$$

The *canonical elementary differential* $\theta(\rho\tau)$ is defined as follows. Choose a labeled representative $\rho\lambda\tau$ of $\rho\tau$ in which the root is labeled with 1.

Definition 3.1 *The canonical elementary differential associated with a rooted tree of order $r \geq 2$ is given by*

$$\theta(\rho\tau) \ = \ \sum_{j_2} \cdots \sum_{j_r} H_{c(1)}\, F^{j_2}_{c(2)} \cdots F^{j_r}_{c(r)} \ ,$$

where superscripts denote vector components of the elementary differentials $\mathbf{F} = \mathbf{F}(\rho\tau)$. The subscripts $c(i) = j_{s_1(i)} j_{s_2(i)} \ldots j_{s_k(i)}$ are multi-indices given by the labels $s_1(i), \ldots, s_k(i)$ of all sons of the vertex with label i. They denote differentiation with respect to the corresponding components of the vector $\mathbf{y} = (\mathbf{q}, \mathbf{p})^T$.

It was proven in [8] that the canonical elementary differentials only change in sign under root-shifting:

$$\theta(\rho\tau_1) \ = \ (-1)^L\, \theta(\rho\tau_2) \ ,$$

where $\rho\tau_1$,$\rho\tau_2 \in \tau$ are rootings of the same tree τ and L is the length of the path between the roots. In particular, for superfluous trees the associated canonical elementary differentials vanish identically. Hence one can omit all contributions from superfluous trees, denoted by $\tau \notin sup$. We then group different rootings of trees corresponding to the same parity in (3.6) to obtain

$$\frac{\partial^{r-1}\Gamma}{\partial h^{r-1}} = -\frac{1}{r} \sum_{\substack{\tau \notin sup \\ r(\tau)=r}} \left(\sum_1 \alpha(\rho\tau)\,\gamma(\rho\tau)\,\Phi(\rho\tau) - \sum_2 \alpha(\rho\tau)\,\gamma(\rho\tau)\,\Phi(\rho\tau) \right) \theta_1(\tau) \tag{3.7}$$

for $r \geq 2$. The sums $\sum_1$ and $\sum_2$ extend to all rooted representatives in the two parity classes of τ. By θ_1 we denote the (common) corresponding elementary differential associated with $\sum_1$.

4 Simplifying the canonical elementary coefficients.

Recall from [11] that $\tilde{\Phi}$ and $\tilde{\delta}$ are the analogues of weight and the reciprocal of density. These are formed by eliminating the symplecticity condition via the parametrisation (3.3). In particular we have

$$\Phi(\rho\tau) - \frac{1}{\gamma(\rho\tau)} \;=\; \tilde{\Phi}(\rho\tau) - \tilde{\delta}(\rho\tau) \;+\; o(\rho\tau) \;, \tag{4.1}$$

where $o(\rho\tau)$ is an expression involving only subtrees of lower order. If the order conditions

$$\Phi(\rho\tau') \;=\; \frac{1}{\gamma(\rho\tau')} \;, \quad \text{or equivalently,} \quad \tilde{\Phi}(\rho\tau') \;=\; \tilde{\delta}(\rho\tau')$$

are satisfied for all rooted trees $\rho\tau'$ of order $r' < r$, then $o(\rho\tau) = 0$ for any rooted tree of order r. As for the canonical elementary differentials, the new weight and density have the crucial property that they only change in sign under root-shifting:

$$\tilde{\Phi}(\rho\tau_1) = (-1)^L \; \tilde{\Phi}(\rho\tau_2) \;, \quad \tilde{\delta}(\rho\tau_1) = (-1)^L \; \tilde{\delta}(\rho\tau_2) \;,$$

where $\rho\tau_1$ and $\rho\tau_2$ arise from the same tree τ and differ only in the location of the root. The integer L is the length of the path between the roots.

We re-write (3.7) in terms of the new formalism involving $\tilde{\Phi}$ and $\tilde{\delta}$. Assume that the order conditions hold for all trees $\rho\tau'$ of order $r' < r$. Then

$$\begin{aligned}
&\frac{\partial^{r-1}\Gamma}{\partial h^{r-1}} \\
&\stackrel{a)}{=} \frac{1}{r} \sum_{\substack{\tau\notin sup \\ r(\tau)=r}} \left(\sum_2 \alpha(\rho\tau) \left(\gamma(\rho\tau)\; \Phi(\rho\tau) - 1\right) - \sum_1 \alpha(\rho\tau) \left(\gamma(\rho\tau)\; \Phi(\rho\tau) - 1\right) \right) \; \theta_1(\tau) \\
&\stackrel{b)}{=} \frac{1}{r} \sum_{\substack{\tau\notin sup \\ r(\tau)=r}} \left(\sum_2 \alpha(\rho\tau)\; \gamma(\rho\tau) \left(\tilde{\Phi}(\rho\tau) - \tilde{\delta}(\rho\tau)\right) - \sum_1 \alpha(\rho\tau)\; \gamma(\rho\tau) \left(\tilde{\Phi}(\rho\tau) - \tilde{\delta}(\rho\tau)\right) \right) \; \theta_1(\tau) \\
&\stackrel{c)}{=} \sum_{\substack{\tau\notin sup \\ r(\tau)=r}} \left(\frac{1}{r} \sum_{\rho\tau\in\tau} \alpha(\rho\tau)\; \gamma(\rho\tau) \right) \left(\tilde{\delta}(\rho\tau_0) - \tilde{\Phi}(\rho\tau_0)\right) \; \theta(\rho\tau_0).
\end{aligned}$$

For a) we note the result

$$\sum_1 \alpha(\rho\tau) = \sum_2 \alpha(\rho\tau)$$

taken from [8]. For b) we use (4.1) with $o(\rho\tau) = 0$, since the order conditions for lower order trees are assumed. For c) the root-shifting properties of $\tilde{\Phi}$ and $\tilde{\delta}$ are used to factor the sums. The product $(\tilde{\delta} - \tilde{\Phi})\,\theta$ has a common value for all rooted trees in τ, so that any rooted representative $\rho\tau_0$ of τ may be used.

This re-formulation of the results in [8] clearly shows that only one order condition per non-superfluous, non-rooted tree is involved in the derivation of symplectic Runge-Kutta schemes. The only term involving different rootings of the tree is the factor

$$\hat{\beta}(\tau) \;=\; \frac{1}{r(\tau)} \sum_{\rho\tau\in\tau} \alpha(\rho\tau)\,\gamma(\rho\tau)\;. \tag{4.2}$$

With the notation of section 2

$$\alpha(\rho\tau)\,\gamma(\rho\tau) \;=\; r(\tau)\,\beta(\rho\tau) \;=\; \bar{\beta}(\rho\tau) \;=\; \frac{r(\tau)\,!}{\sigma(\rho\tau)} \;=\; \frac{r(\tau)\,!\,\varsigma(\rho\tau)}{\sigma(\tau)}$$

and one obtains the following interpretation of this factor:

$$\hat{\beta}(\tau) \;=\; \sum_{\rho\tau\in\tau} \beta(\rho\tau) \;=\; \frac{\bar{\beta}(\rho\tau_0)}{\varsigma(\rho\tau_0)} \;=\; \frac{r(\tau)\,!}{\sigma(\tau)}\;.$$

We note that the quotient $\bar{\beta}(\rho\tau)/\varsigma(\rho\tau) = r(\tau)!/\sigma(\tau)$ is independent of the rooting of the tree, so that any representative $\rho\tau_0 \in \tau$ may be chosen. Further, we have used

$$\sum_{\rho\tau\in\tau} \varsigma(\rho\tau) \;=\; \sum_{\rho\in V} 1 \;=\; r(\tau)\;,$$

where $\varsigma(\rho\tau)$ summarises all identical rooted trees obtained when systematically shifting the root ρ to all vertices of τ.

With this result we may finally express the coefficients (4.2) in terms of only one rooted candidate $\rho\tau_0$ per tree, so that for $r \geq 2$,

$$\frac{\partial^{r-1}\Gamma}{\partial h^{r-1}} \;=\; \sum_{\substack{\tau\notin sup\\ r(\tau)=r}} \frac{\bar{\beta}(\rho\tau_0)}{\varsigma(\rho\tau_0)} \left(\tilde{\delta}(\rho\tau_0) - \tilde{\Phi}(\rho\tau_0)\right)\,\theta(\rho\tau_0)\;. \tag{4.3}$$

¿From example 2.2, if we choose $\rho\tau_0$ as a centroid, $\varsigma(\rho\tau) = 1$ and (4.3) is simplified further.

5 Conclusions.

In [11] we demonstrated how to derive a new order condition framework for symplectic Runge-Kutta schemes. Different rooted trees then give rise to the same algebraic constraint. Here we have shown that the canonical elementary differential can also be specified in terms of only one rooted candidate per tree.

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