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RUNGE–KUTTA METHODS ADAPTED TO MANIFOLDS AND BASED ON RIGID FRAMES *

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Abstract.

We consider numerical integration methods for differentiable manifolds as proposed by Crouch and Grossman. The differential system is phrased by means of a system of frame vector fields $E_1, \ldots, E_n$ on the manifold. The numerical approximation is obtained by composing flows of certain vector fields in the linear span of $E_1, \ldots, E_n$ that are tangent to the differential system at various points. The methods reduce to traditional Runge-Kutta methods if the frame vector fields are chosen as the standard basis of euclidean $\mathbb{R}^n$. A complete theory for the order conditions involving ordered rooted trees is developed. Examples of explicit and diagonal implicit methods are presented, along with some numerical results.

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1 Introduction

Consider the initial value problem

$$\dot{y} = f(t, y), \quad y(0) = y_0, \quad f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n. \tag{1.1}$$

Such and similar openings have been fairly common in papers within the field of numerical ODEs for many years. For readers who normally solve differential equations in the vector space $\mathbb{R}^n$, (1.1) is of course an excellent point of departure. Those whose problems are phrased on a differentiable manifold M may still be happy with the formulation (1.1), since a manifold by definition has a local representation in $\mathbb{R}^n$ for some n. Certainly, there may be difficulties when the numerical method needs to switch from one coordinate chart to another, but experience will perhaps reveal that this is not a serious obstacle in most

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practical problems. It is possibly a more serious difficulty that for many manifolds, the local coordinate charts may be complicated and that the derivation of a representation of the form (1.1) may call for lengthy calculations by hand or by a computer algebra system. In many such cases it is preferable to embed the manifold in $\mathbb{R}^N$ for some $N > n$. This may lead to simpler expressions, and the representation can be made global. But a difficulty that arises here is that the computed solution may drift off the manifold unless information about it is encoded in the algorithm. Recently, some authors like Crouch and Grossman [3], and Munthe-Kaas with coauthors [10, 11, 12] have adopted a different view on differential equations on manifolds, taking one step up the ladder of abstraction. Rather than introducing coordinates already in the definition of the differential equation, like in (1.1), the solution to the ODE is considered as a smooth curve on the manifold and the differential equation is interpreted as a vector field for which this smooth curve is an integral curve. The integration method is then formulated in this abstract setting. It should be emphasized that our motivation for this approach is not to develop a more general type of method, but rather the opposite; to tailor integration methods by allowing the user to take into consideration the particular manifold on which the solution is known to evolve. The method is designed such that the numerical approximation may be forced to evolve on the manifold by means of flows of certain vector fields. The methods proposed by Munthe-Kaas are phrased in the most general case for homogeneous manifolds, see [12], and he also shows that the methods by Crouch and Grossman [3] can be interpreted in the setting of such manifolds. Perhaps the most important examples of homogeneous manifolds are the Lie groups. The configuration of a suspended rigid body can be thought of as an element of the Lie group, $SO(3)$, the group of rotations in three dimensions. Hence, many applications can be found for instance within the field of structural dynamics.

An important class of differential equations on manifolds are the differential-algebraic problems. One may for instance have a set of algebraic equations that define the manifold as an embedding in a higher dimensional vector space. In such a case, it may appear natural to look for a system of vector fields in involution that spans the tangent bundle of this manifold. A numerical method for such a problem may then typically use as primitives flows of these vector fields.

In this paper we shall study the approach proposed by Crouch and Grossman in [3] and applied to a problem in mechanics in [4]. They develop methods for manifolds both as generalizations of multistep methods and Runge-Kutta methods. Here we will focus on the latter type, and give a complete description of the conditions that must be imposed by the method coefficients to ensure that the order of consistency is equal to a given integer. We begin in Section 2 by introducing some necessary notation and present the format of the methods. In Section 3, we introduce the concept of ordered rooted trees and we consider their connection to the Lie series of the exact solution. By developing the numerical solution in a similar series, we obtain in Section 4 a characterization of the order conditions. It turns out that the conditions are not all independent, and we present a way of reducing them to a minimal set in Section 5. In Section 6, we present a few examples of Crouch-Grossman methods, to our knowledge the first explicit one of order 4. Finally, we show how the methods work for Lie groups, and pay special attention to the case of matrix groups. We give numerical examples to demonstrate that the order theory is correct for the spinning top problem.

2 Background and notation

We introduce only the concepts from differential geometry that are strictly necessary for the discussion that follows. The reader may find that the text by Warner [18] is quite compatible with the notation used here.

Let M be a differentiable manifold. A tangent vector v at the point $p \in M$ is a linear derivation, acting on functions on M, such that for any $f, g \in C^\infty(M, \mathbb{R})$ and $\lambda \in \mathbb{R}$

$$\begin{aligned} v[f + \lambda g] &= v[f] + \lambda v[g] \\ v[f \cdot g] &= f(p)v[g] + g(p)v[f] \qquad \text{(Leibniz' rule).} \end{aligned}$$

The set of all tangent vectors to M at p is called the *tangent space to M at p*, and is denoted TM_p. It can be imposed the structure of a vector space in the natural way, in fact, with a choice of local coordinates, say $(x_1, \ldots, x_n)$, a tangent vector v can be expressed as

$$v = v_1 \frac{\partial}{\partial x_1} + v_2 \frac{\partial}{\partial x_2} + \cdots + v_n \frac{\partial}{\partial x_n}.$$

Thus, a tangent vector v can be associated with a direction $(v_1, \ldots, v_n) \in \mathbb{R}^n$ and we can think of its action on f at p as the rate of change in f from p along this direction.

The *tangent bundle* of M is defined as

$$TM = \bigcup_{p \in M} TM_p.$$

A differentiable structure on TM is induced in a natural way from that of M. A *vector field* F on M is a section of TM, i.e.

$$\begin{aligned} F: \quad M &\to TM \\ p &\mapsto v(p), \quad v(p) \in TM_p. \end{aligned}$$

If $\phi : M \to N$ is a C^∞ map between the two manifolds M and N, we define the differential of ϕ at the point p to be the linear map $d\phi : TM_p \to TN_{\phi(p)}$

$$d\phi(v)[g] = v[g \circ \phi], \quad v \in TM_p \text{ and } g \in C^\infty(N, \mathbb{R}).$$

A smooth curve on M is a C^∞ map $\sigma : (a, b) \to M$ where (a, b) is an interval. The tangent vector of σ at $t = t_0$ is an element, $\dot\sigma(t_0) \in TM_{\sigma(t_0)}$, given as

$$\dot\sigma(t_0) = d\sigma \left(\left. \frac{d}{dt} \right|_{t_0} \right).$$

We may interpret this in coordinates $(x_1, \dots, x_n)$ as

$$\dot\sigma(t_0) = \sum_{i=1}^{n} \left.\frac{d(x_i \circ \sigma)}{dt}\right|_{t_0} \frac{\partial}{\partial x_i}.$$

A smooth curve $\sigma(t)$ is an *integral curve* of a vector field F if

$$\dot\sigma(t) = F(\sigma(t)), \quad t \in (a, b).$$

If F is a smooth vector field on M, then there exists, for each $p \in M$, an interval $(a(p), b(p))$ and a smooth curve, $\sigma_p : (a(p), b(p)) \to M$ with $\sigma(0) = p$ such that $\sigma_p(t)$ is an integral curve of F. Now, fixing t, we can obtain a diffeomorphism of M by setting

$$\begin{aligned} \phi_{F,t} \quad : \quad & \mathfrak{D}_t \to M, \quad \text{where} \quad \mathfrak{D}_t = \{p \in M : t \in (a(p), b(p))\} \\ & p \mapsto \sigma_p(t). \end{aligned}$$

This map is called *the flow* of the vector field F.

Let $E_1, \dots, E_n$ be smooth vector fields on M. In the obvious way, they generate a vector space, $\mathcal{V}$ over $\mathbb{R}$, and a module, Ω over the ring $C^\infty(M, \mathbb{R})$. In what follows, we shall be interested in approximating flows of vector fields in Ω with flows of vector fields in $\mathcal{V}$. Notice that for any $F \in \Omega$ and $p \in M$ we can associate a vector field $F_p \in \mathcal{V}$ *with frozen coefficients relative to the frame vector fields* $E_1, \dots, E_n$ where

$$F_p = \sum_{i=1}^{n} f_i(p) E_i.$$

For any vector field F in either Ω or $\mathcal{V}$ we shall use the notation

$$\phi_{F,t}(p) =: e^{tF}\, p = \exp(tF)p$$

for its flow. By a system of differential equations relative to the vector fields $E_1, \dots, E_n$, we shall mean an equation of the form

$$\dot y = F(y) = \sum_{i=1}^{n} f_i(y) E_i, \quad y(0) = y_0, \quad F \in \Omega, \tag{2.1}$$

whose solution is an integral curve $y : [0, T] \to M$ of F. It is well known that for a function $\psi \in C^\infty(M, \mathbb{R})$ and $h \in \mathbb{R}$, the composition $\psi \circ e^{hF} p$ has a Lie series

$$\psi(p) + hF[\psi](p) + \frac{1}{2}h^2 F^2[\psi](p) + \cdots + \frac{1}{r!}h^r F^r[\psi](p) + \cdots \tag{2.2}$$

where we use the convention $F^{r+1}[\psi] = F\left[F^r[\psi]\right]$, $r = 1, 2, \dots$. Observe that the operator F^r, $r \geq 2$, will not normally be a vector field, actually it can be regarded as a map $p \mapsto v^r(p)$ with $v^r(p) \in TM_p^r$, the vector space of rth order tangent vectors at p. With a choice $x_1, \ldots, x_n$ of local coordinates, a basis for TM_p^r is

$$\left\{ \left.\frac{\partial^\alpha}{\partial x^\alpha}\right|_p : 1 \le |\alpha| \le r \right\}, \quad \text{where} \quad \alpha = (\alpha_1, \ldots, \alpha_n) \quad \text{and} \quad |\alpha| = \sum_{i=1}^n \alpha_i.$$

Clearly one has $TM_p = TM_p^1 \subset TM_p^2 \subset \cdots$. The union $\bigcup_p TM_p^r$ is called the rth tangent bundle of M.

Crouch and Grossman propose to approximate the solution of (2.1) by a generalization of explicit Runge-Kutta methods, under the assumption that flows of vector fields in $\mathcal{V}$ can be computed. In this paper, we also allow for the methods to be implicit, hence we propose a procedure as follows

$$\begin{aligned} p &= y_k, && \\ Y_r &= e^{ha_{r,s}F_p^s} \circ \cdots \circ e^{ha_{r1}F_p^1}\, p && r = 1, \ldots, s \\ F_p^r &= F_{Y_r} = \sum_{i=1}^n f_i(Y_r)\, E_i && r = 1, \ldots, s \\ y_{k+1} &= e^{hb_s F_p^s} \circ e^{hb_{s-1}F_p^{s-1}} \circ \cdots \circ e^{hb_1 F_p^1}\, p. && \end{aligned} \tag{2.3}$$

The scheme is well defined for sufficiently small values of the step size h. As it is implicit, both in the approximations $Y_r \in M$ and the vector fields $F_p^r \in \mathcal{V}$, one needs a procedure for the solution of such equations on manifolds. As of yet, it is not clear to us how this should be accomplished for general differentiable manifolds. However, in a recent paper by Owren and Welfert [14] a version of the Newton iteration is proposed in the case that M is a Lie group. We will subsequently refer to methods of the format (2.3) as *Crouch-Grossman methods*.

Note that the notation for the coefficients of the method (a_{rj}) and (b_r) is consistent with the usual Runge-Kutta methods, and hence they can be represented in a Butcher tableau. We will subsequently refer to the coefficients c_r, $r = 1, \ldots, s$, where $c_r = \sum_{j=1}^s a_{rj}$.

Also, as pointed out in [3], the method reduces to a traditional Runge-Kutta method if the manifold is the vector space $\mathbb{R}^n$ and the vector fields E_i are chosen as the standard euclidean basis. To see this, let $(x_1, \ldots, x_n)$ be coordinates on $\mathbb{R}^n$ and let the frame vector fields be defined as $E_i : y \mapsto \partial/\partial x_i|_y$, $1 \le i \le n$. For $q \in \mathbb{R}^n$ we let $F_q : y \mapsto \sum f_i(q)\, \partial/\partial x_i|_y$. We then find that $\exp(aF_q)\, p = p + af(q)$, where $a \in \mathbb{R}$ and $f(q) = (f_1(q), \ldots, f_n(q))^T$. By applying this repeatedly to the formulas in (2.3) we recover the usual Runge-Kutta method.

The method defined by (2.3) is a one-step method, hence we can write $y_{k+1} = \Psi(h, y_k) = \Psi(h, p)$. The order of such a method can be defined as the greatest integer q for which

$$\left.\frac{d^r}{dh^r}\left(\psi \circ e^{hF} p\right)\right|_{h=0} = \left.\frac{d^r}{dh^r}\left(\psi \circ \Psi(h,p)\right)\right|_{h=0}, \quad r = 0, \ldots, q, \quad \forall\ \psi \in C^\infty(M, \mathbb{R}), \tag{2.4}$$

and note again that this definition of order is consistent with the usual definition when the frame vector fields are chosen as the standard euclidean basis.

3 Trees and their relation to the Lie series of the exact solution

We begin by quoting a definition from [6] for labelled rooted trees.

DEFINITION 3.1. *Let A be an ordered chain of indices $A = \{r < i_1 < i_2 < \cdots\}$ and denote by A_q the subset consisting of the first q indices. A* (rooted) labelled tree of order q *is a mapping*

$$t : A_q \backslash \{r\} \to A_q \qquad \text{such that } t(z) < z \; \forall \; z \in A_q \backslash \{r\}.$$

The set of labelled trees of order q is denoted LT^q.

While this definition is the same as in the classical case, we need to modify the concept of equivalence classes of labelled trees as defined in [6].

DEFINITION 3.2. *Two labelled trees t and u are equivalent if they have the same order, say q, and if there exists a permutation $\sigma : A_q \to A_q$ such that*

1. $\sigma(r) = r$
2. $t\sigma = \sigma u$ *on* $A_q \backslash \{r\}$
3. *for all* $z_1, z_2 \in A_q \backslash \{r\}$ *such that* $t(z_1) = t(z_2)$,

$$\sigma(z_1) < \sigma(z_2) \Leftrightarrow z_1 < z_2.$$

The equivalence classes induced by this relation are called ordered (rooted) trees (T_O^q). *The number of labelled rooted trees belonging to an equivalence class $t \in T_O^q$ is denoted $\alpha(t)$. The set of all rooted trees is $T_O = T_O^1 \cup T_O^2 \cup \cdots$. The function $\rho : T_O \to \mathbb{Z}^+$ is defined as $\rho(t) = q$ if $t \in T_O^q$.*

DEFINITION 3.3. *The set of special ordered (rooted) trees S_O^q with q nodes is defined as follows.*

1. $S_O^q \subseteq T_O^q$
2. *A tree $\hat{s} \in LT^q$ belongs to an equivalence class of $s \in S_O^q$ if and only if the set $\hat{s}^{-1}(\{z\})$ contains at most one element for all $z \in A_q \backslash \{r\}$. In other words, S_O^q is the set of all ordered trees, with exactly q nodes, that have no ramifications except at the root.*

There is a more convenient notation for ordered rooted trees. We denote the trivial one-node tree τ and write any ordered tree with two or more nodes on the form $t = [t_1, \ldots, t_\mu]$. Such a tree is obtained by adjoining each root of the trees $t_1, \ldots, t_\mu$ to a new node that becomes the root of t. Of course, the ordering of the trees in the bracket is now significant, the chosen convention being that for all labelled trees which correspond to the ordered tree $t = [t_1, \ldots, t_\mu]$ we have $i < j \Rightarrow r_i > r_j$, where r_k is the index of the root of t_k.

It is well known (see e.g. [2]) that the number of ordered trees with exactly r nodes is equal to the Catalan number

$$N_r = \frac{1}{r}\binom{2r-2}{r-1}.$$

As for the number of labelled trees, $\alpha(t)$, belonging to an equivalence class $t \in T_O^\rho$ we have the following recursion formula.

PROPOSITION 3.1. *$\alpha(\tau) = 1$. Let $t \in T_O^\rho$ be of the form $t = [t_1, t_2, \ldots, t_\mu]$ where each subtree t_i has ρ_i nodes. Then*

$$\alpha(t) = \prod_{\ell=1}^{\mu} \binom{\sum_{i=1}^{\ell} \rho_i - 1}{\rho_\ell - 1} \alpha(t_\ell).$$

PROOF. $\alpha(\tau) = 1$ is obvious. We must consider the number of ways to distribute $\rho = 1 + \sum_{i=1}^{\mu} \rho_i$ indices that are eligible according to Definition 3.2. Clearly, the two smallest indices must be assigned to the roots of t and t_μ respectively. There are now $\binom{\rho-2}{\rho_\mu - 1}$ ways to choose the remaining $\rho_\mu - 1$ nodes of t_μ and these can be distributed internally on t_μ in $\alpha(t_\mu)$ ways. If $\mu > 1$ we must proceed by assigning to the root of $t_{\mu-1}$ the smallest of the remaining indices. There are then $\rho_{\mu-1}$ indices to choose from the remaining $\rho - 2 - \rho_\mu$ indices. This argument is used iteratively along with the relation $\rho = 1 + \sum_{i=1}^{\mu} \rho_i$ to yield the required result. □

We now proceed to establish the correspondence between the set of ordered trees and a counterpart to *the elementary differentials* known from the classical theory of Runge-Kutta methods. These constitute the terms obtained from the powers of the vector field F in (2.2). We compute the first few powers of F using only Leibniz' rule and linearity of the vector fields E_i.

$$F^1 = F = \sum_{i_1} f_{i_1} E_{i_1},$$

$$F^2 = \sum_{i_1, i_2} \left(f_{i_2} f_{i_1} E_{i_2} E_{i_1} + f_{i_2} E_{i_2}[f_{i_1}] E_{i_1} \right),$$

$$\begin{aligned} F^3 = \sum_{i_1,i_2,i_3} \Big(& \overset{(1)}{f_{i_3} f_{i_2} f_{i_1} E_{i_3} E_{i_2} E_{i_1}} + \overset{(2)}{f_{i_3} f_{i_2} E_{i_3}[f_{i_1}] E_{i_2} E_{i_1}} + \overset{(3)}{f_{i_3} E_{i_3}[f_{i_2}] f_{i_1} E_{i_2} E_{i_1}} \\ & + \overset{(4)}{f_{i_3} f_{i_2} E_{i_2}[f_{i_1}] E_{i_3} E_{i_1}} + \overset{(5)}{f_{i_3} E_{i_3}[f_{i_2}] E_{i_2}[f_{i_1}] E_{i_1}} + \overset{(6)}{f_{i_3} f_{i_2} E_{i_3} E_{i_2}[f_{i_1}] E_{i_1}} \Big). \end{aligned}$$

It is natural to identify the expression for F^1 with the 2-node tree in Figure 3.1. Similarly, we identify the two terms of F^2 with the two 3-node trees. In F^3 there are six terms, each corresponding to a labelled rooted tree with 4 nodes in the figure below. Terms 2 and 4 correspond to the labelled trees depicted in the frame. They only differ in the sense that the indices i_2 and i_3 are interchanged. But term 3 is in general different since $E_{i_1} E_{i_2} \neq E_{i_2} E_{i_1}$ whenever $i_1 \neq i_2$. Thus, when identifying a labelled tree with a term in F^q one must make sure that the order in the composition of frame vector fields $E_{i_j} E_{i_k} \cdots$ is retained, above we use the convention that the labels should be decreasing from left to right.

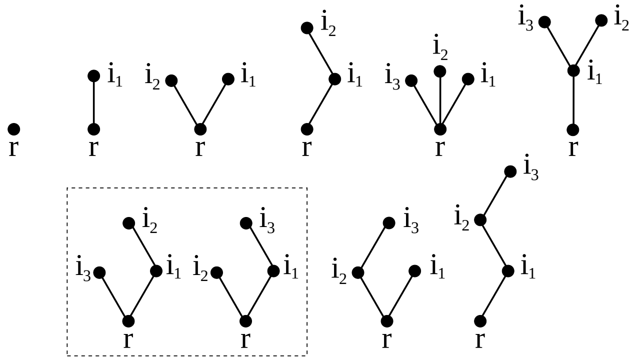

Figure 3.1: Labelled rooted trees with $q \leq 4$

We see that the result of applying F (differentiation) to an elementary differential is that a new branch is added at each node, introducing a new greater label. In this way we find that there is a one-to-one correspondence between the set of labelled trees with $\rho(t)$ nodes and the set of elementary differentials constituting the differential operator $F^{\rho(t)-1}$. To see this correspondence when drawing the labelled trees in a diagram, it may be helpful to always add the new branch to the left in each ramification (although no such distinction is made in the definition of a labelled tree).

DEFINITION 3.4. *We define the elementary differentials, relative to the frame vector fields $E_1, \ldots, E_n$ in the following way.*

$$\begin{aligned} \mathbb{F}(\tau) &= \mathbb{1}, \\ \mathbb{F}([t_1, \ldots, t_\mu]) &= \sum_{i_1, \ldots, i_\mu} \mathbb{F}(t_1)[f_{i_1}] \cdot \mathbb{F}(t_2)[f_{i_2}] \cdots \mathbb{F}(t_\mu)[f_{i_\mu}]\, E_{i_1} E_{i_2} \cdots E_{i_\mu}, \end{aligned}$$

where $\mathbb{1}$ denotes the identity operator. We find that

$$\psi \circ e^{hF} p = \sum_{t \in T_O} \frac{h^{\rho(t)-1}}{(\rho(t)-1)!}\, \alpha(t)\, \mathbb{F}(t)[\psi](p), \tag{3.1}$$

which is similar to the classical theory.

Notice that due to the structure of the elementary differentials, we have that for any $t \in T_O$ of the form $t = [t_1, \ldots, t_\mu]$,

$$\mathbb{F}(t)[\psi](p) = \sum_{i_1, \ldots, i_\mu} \mathbb{F}(t_1)[f_{i_1}](p) \cdots \mathbb{F}(t_\mu)[f_{i_\mu}](p) E_{i_1} \cdots E_{i_\mu}[\psi](p),$$

and for this reason we define the *frozen elementary differentials* $\mathbb{F}_p(t)$ by

$$\begin{aligned}\mathbb{F}_p(\tau) &= \mathbb{1},\\ \mathbb{F}_p([t_1,\dots,t_\mu]) &= \sum_{i_1,\dots,i_\mu} \mathbb{F}(t_1)[f_{i_1}](p)\cdot\mathbb{F}(t_2)[f_{i_2}](p)\cdots\mathbb{F}(t_\mu)[f_{i_\mu}](p)\, E_{i_1}E_{i_2}\cdots E_{i_\mu}.\end{aligned}$$

In particular,

$$\mathbb{F}_p([\tau]) = \sum_{i_1}\mathbb{F}(\tau)[f_{i_1}](p)E_{i_1} = \sum_{i_1} f_{i_1}(p)E_{i_1}.$$

Clearly, from (3.1) we must have

$$\frac{d^q}{dh^q}\left(\psi\circ e^{hF}p\right)\Big|_{h=0} = \sum_{t\in T_O^{q+1}} \alpha(t)\mathbb{F}_p(t)[\psi](p), \quad q=0,1,\dots \tag{3.2}$$

REMARK 3.1. *In (3.2) the qth derivative of the exact solution is related to ordered trees with $q+1$ nodes, contrary to the classical theory where the qth derivative corresponds to trees with only q nodes. The restriction of our approach to the euclidean case amounts to choosing coordinate functions $\phi_i : y \to y_i$, and frame vector fields $E_i : y \mapsto \partial/\partial y_i$. By applying the elementary differential (operator) to ψ_i, we find that all $\mathbb{F}_p(t)$ vanish when t is of the form $[t_1,\dots,t_\mu]$ with $\mu \geq 2$. We are left simply with the $\mathbb{F}_p(t)$ corresponding to trees of the form $t=[u]$, hence by identifying each such t with u we obtain a representation of $F^{\rho(t)}$ by means of trees with $\rho(t)$ nodes.*

4 The derivatives of the approximate solution

We need to find expressions for the rth derivative of $\psi\circ\Psi(h,p)$ as it occurs in (2.4). This can be done in different ways, one of them is proposed in [3]. Another technique is based on the use of the Baker-Campbell-Hausdorff formula [17], i.e., the composition of flows occurring in (2.3) can be replaced by the flow of one single vector field, say $G(h)$. Then $\exp(G(h))$ can be differentiated with respect to h through the introduction of the differential of the exponential map. Although this approach is straightforward, it seems to generate extremely long and complicated expressions involving iterated Lie brackets of vector fields, and we have not been able to discover any tractable way of dealing with them. Instead, we have chosen to base the expansion of the numerical approximation solely on ordered rooted trees arising from the use of Lie series, not very unlike the expansion of the exact solution as given in the previous section. This results in a nice and clean theory, and it is consistent with the theory for classical Runge-Kutta methods. A disadvantage is that one obtains several redundant conditions, such that only a subset of them needs to be considered. We present in the next section some results that can be used to select those conditions that can be discarded.

Let $j = (j_1, \dots, j_r)$ be a multi-index of integer elements with $1 \le j_r \le s$. We define

(4.1)
$$j! := q_1! q_2! \cdots q_s!, \quad \text{where } q_i \text{ is the number of occurrences of } i \text{ in } (j_1, \dots, j_r).$$

For example, with $j = (1, 1, 2, 3, 3)$ we have $j! = 2! \cdot 1! \cdot 2! = 4$.

We have the following result.

Lemma 4.1. *For any real s-tuple $v = (v_1, \dots, v_s)$, $\psi \in C^\infty(M, \mathbb{R})$, and smooth vector fields $F_p^1, \dots, F_p^s \in \mathcal{V}$ depending on h, the composition of their flows is defined for sufficiently small values of h and can be written as follows*

$$\psi\big(e^{hv_s F_p^s} \circ \cdots \circ e^{hv_1 F_p^1}\, p\big) = W_v(h)[\psi](p)$$

where $W_v(h)$ is the formal operator

$$W_v(h) = \mathbb{1} + \sum_{r=1}^{\infty} h^r \sum_{j_1=1}^{s} \sum_{j_2=j_1}^{s} \cdots \sum_{j_r=j_{r-1}}^{s} \frac{1}{j!} v_{j_1} \cdots v_{j_r}\, F_p^{j_1} \cdots F_p^{j_r}. \tag{4.2}$$

Furthermore, there is a Faà di Bruno type of formula for the qth derivative of the operator $W_v(h)$,

$$W_v^{(q)}(h)\Big|_{h=0} = \sum_{u \in S_O^{q+1}} \frac{q!}{\prod_{\nu=1}^{\mu} (\delta_\nu - 1)!} \times \sum_{1 \le j_1 \le \cdots \le j_\mu \le s} \frac{1}{j!} v_{j_1} \cdots v_{j_\mu}\, \big(F_p^{j_1}\big)^{(\delta_1 - 1)} \cdots \big(F_p^{j_\mu}\big)^{(\delta_\mu - 1)}\Big|_{h=0},$$

for $q = 1, 2, \dots$. Here, $u \in S_O^{q+1}$ is of the form $[u_1, \dots, u_\mu]$ and $\delta_i = \rho(u_i)$ (compare [6, Lemma 2.8 (p. 150)])

Proof. We compute

$$\psi(e^{hv_s F_p^s} \circ \cdots \circ e^{hv_1 F_p^1}\, p)$$

by using formula (2.2) repeatedly, beginning with $F = v_s F_p^s$ and p replaced by $e^{v_{s-1} F_p^{s-1}} \circ \cdots \circ e^{hv_1 F_p^1}\, p$.

This leads to the expression

$$\sum_{r_1=0}^{\infty} \cdots \sum_{r_s=0}^{\infty} \frac{h^r}{r_1! \cdots r_s!} v_1^{r_1} \cdots v_s^{r_s}\, \big(F_p^1\big)^{r_1} \cdots \big(F_p^s\big)^{r_s}\, [\psi](p),$$

where $r = r_1 + \cdots + r_s$, which is equal to $W_v(h)[\psi](p)$.

For sufficiently small h we can do a term-wise differentiation of $W_v(h)$, and we recall the formula

$$(h^r\, g(h))^{(q)}\Big|_{h=0} = \begin{cases} 0 & \text{if } q < r \\ \dfrac{q!}{(q-r)!} g(h)^{(q-r)}\Big|_{h=0} & \text{if } q \ge r \end{cases}$$

for any smooth function $g(h)$. We shall apply this formula to (4.2). Repeated use of Leibniz' rule yields

$$\left(F_p^{j_1}\cdots F_p^{j_r}\right)^{(q-r)} = \sum_{\delta_1+\cdots+\delta_r=q} \binom{q-r}{\delta_1-1,\dots,\delta_r-1} \left(F_p^{j_1}\right)^{(\delta_1-1)}\cdots\left(F_p^{j_r}\right)^{(\delta_r-1)}.$$

Any ordered r-plet $(\delta_1,\dots,\delta_r)$ identifies uniquely a term in the $(q-r)$th derivative of

$$\sum_{1\le j_1\le\cdots\le j_r\le s} \frac{1}{j!}\left(F_p^{j_1}\cdots F_p^{j_r}\right)^{(q-r)}.$$

On the other hand, the same r-plet identifies uniquely the tree $u\in S_O^{q+1}$ with subtrees u_i such that $\rho(u_i)=\delta_i$. Thus, by summing over all trees in S_O^{q+1} we obtain the last part of the lemma. □

We have the following main result for the derivatives of the approximate solution.

THEOREM 4.2. *For a given Crouch-Grossman method (2.3), let* $\Phi_r : T_O \to \mathbb{R}$ *be defined recursively for each* $r=1,\dots,s$ *as*

$$\begin{aligned} \Phi_r(\tau) &= 1, \qquad \textit{and for } t=[t_1,\dots,t_\mu] \\ \Phi_r(t) &= \sum_{j_1=1}^{s}\sum_{j_2=j_1}^{s}\cdots\sum_{j_\mu=j_{\mu-1}}^{s}\frac{1}{j!}\,a_{r,j_1}\cdots a_{r,j_\mu}\,\Phi_{j_1}(t_1)\cdots\Phi_{j_\mu}(t_\mu), \end{aligned} \tag{4.3}$$

let $\Phi : T_O\to\mathbb{R}$ *be defined as*

$$\begin{aligned} \Phi(\tau) &= 1, \qquad \textit{and for } t=[t_1,\dots,t_\mu] \\ \Phi(t) &= \sum_{j_1=1}^{s}\sum_{j_2=j_1}^{s}\cdots\sum_{j_\mu=j_{\mu-1}}^{s}\frac{1}{j!}\,b_{j_1}\cdots b_{j_\mu}\,\Phi_{j_1}(t_1)\cdots\Phi_{j_\mu}(t_\mu), \end{aligned} \tag{4.4}$$

and let $\gamma : T_O\to\mathbb{Z}^+$ *be defined recursively as*

$$\gamma(\tau)=1, \qquad \gamma(t)=\prod_{r=1}^{\mu}\gamma(t_r)\sum_{i=1}^{r}\rho(t_i) \quad \textit{when } t=[t_1,\dots,t_\mu]. \tag{4.5}$$

Then

$$\left.\frac{d^q}{dh^q}\psi\circ\Psi(h,p)\right|_{h=0} = \sum_{t\in T_O^{q+1}}\alpha(t)\gamma(t)\Phi(t)\mathbb{F}_p(t)[\psi](p), \quad q=1,2,\dots, \tag{4.6}$$

with $\alpha(t)$ *as given in Proposition 3.1.*

It now follows directly from (2.4) and (3.2) that

COROLLARY 4.3. *A Crouch-Grossman method (2.3) is of order* q *if*

$$\Phi(t)=\frac{1}{\gamma(t)} \quad \textit{for all } t\in T_O^2\cup T_O^3\cup\cdots\cup T_O^{q+1}. \tag{4.7}$$

REMARK 4.1. *Note that Corollary 4.3 provides sufficient conditions for a Crouch-Grossman method to have order q. The necessity of these conditions depends on which assumptions that are imposed with respect to the linear independence amongst the elementary differentials* $\left\{\mathbb{F}_p(t) : t \in T_O^2 \cup \cdots \cup T_O^{q+1}\right\}$. *Such assumptions were made with respect to the frame vector fields* $E_1, \ldots, E_n$ *in [3] in order to obtain also necessary order conditions. We shall not make any such assumptions here, but rather leave the choice open to accommodate the application at hand.*

REMARK 4.2. *The reader who is familiar to the classical Butcher theory may be puzzled to observe that the conditions for order q are characterized in terms of trees of orders $2, \ldots, q+1$ rather then $1, \ldots, q$ as in the classical case. Certainly, the coefficients of a Crouch-Grossman method of order q must satisfy the classical order q conditions since the theory is also valid in the case that the frame vector fields coincide with a basis for euclidean* $\mathbb{R}^n$, *i.e.* $E_i : y \mapsto \left.\frac{\partial}{\partial x_i}\right|_y$. *To establish this connection, let* $t = [t_1, \ldots, t_\mu]_{no}$ *be a non-ordered rooted tree, such that* $\rho(t) = q$. *It is possible to show that the classical condition corresponding to t will hold if the order conditions arising from the set of ordered rooted trees*

$$\left\{[[t_{\sigma(1)}, \ldots, t_{\sigma(\mu)}]] \in T_O^{q+1} : \sigma \in S_\mu\right\}$$

are satisfied, where S_μ is the group of permutations on $\{1, \ldots, \mu\}$.

Prior to proving Theorem 4.2 we shall prove the following lemma.

LEMMA 4.4.

$$\alpha(t)\gamma(t) = (\rho(t) - 1)! \quad \textit{for all} \quad t \in T_O.$$

PROOF. $\alpha(\tau)\gamma(\tau) = 1$ by definition. We proceed by induction and assume that the result is true for any $t \in T_O^1 \cup \cdots \cup T_O^{q-1}$ with $q > 1$. Let $t = [t_1, \ldots, t_\mu] \in T_O^q$ and set $\rho_i := \rho(t_i)$. We get from Proposition 3.1 and (4.5)

$$\begin{aligned}
\alpha(t)\gamma(t) &= \prod_{\ell=1}^{\mu}\left(\binom{\sum_{i=1}^{\ell}\rho_i - 1}{\rho_\ell - 1}\sum_{i=1}^{\ell}\rho_i\right)\alpha(t_1)\cdots\alpha(t_\mu)\cdot\gamma(t_1)\cdots\gamma(t_\mu) \\
&= \prod_{\ell=1}^{\mu}\frac{(\sum_{i=1}^{\ell}\rho_i)!}{(\rho_\ell - 1)!(\sum_{i=1}^{\ell-1}\rho_i)!}(\rho_\ell - 1)! = (\rho(t) - 1)!.
\end{aligned}$$

where as usual sums over empty index sets are taken as zero. ◻

PROOF OF THEOREM 4.2. The theorem is proved by induction. We will obtain the auxiliary formula

$$\left.\frac{d^q}{dh^q}(\psi \circ Y_r)\right|_{h=0} = \sum_{t \in T_O^{q+1}} \alpha(t)\gamma(t)\Phi_r(t)\mathbb{F}_p(t), \quad 1 \le r \le s, \quad q = 1, 2, \ldots, \tag{4.8}$$

as a part of the induction proof. In fact, the formula (4.6) can be written in this form if we define $a_{s+1,j} := b_j$, $1 \le j \le s$, $Y_{s+1} := \Psi(h,p)$, and $\Phi_{s+1}(t) := \Phi(t)$. We shall adopt this notation in the rest of the proof. Note also that (4.8) immediately implies

$$\begin{aligned}(F_p^r)^{(q)}\Big|_{h=0} &= \frac{d^q}{dh^q}\Big|_{h=0} \sum_i (f_i \circ Y_r)E_i = \sum_i \sum_{t\in T_O^{q+1}} \alpha(t)\gamma(t)\Phi_r(t)\mathbb{F}_p(t)[f_i]E_i \\ &= \sum_{t\in T_O^{q+1}} \alpha(t)\gamma(t)\Phi_r(t)\mathbb{F}_p([t]). \qquad (4.9)\end{aligned}$$

Let $a_r = (a_{r1}, \ldots, a_{rs})$, $1 \le r \le s+1$. From (2.3) and Lemma 4.1 we find that

$$\psi \circ Y_r = W_{a_r}(h)[\psi], \quad 1 \le r \le s+1,$$

for small h and that

$$\begin{aligned}\frac{d^q}{dh^q}(\psi \circ Y_r)\Big|_{h=0} &= \sum_{u\in S_O^{q+1}} \frac{q!}{\prod_{\nu=1}^{\mu}(\delta_\nu - 1)!} \sum_{j_1=1}^{s} \cdots \sum_{j_\mu=j_{\mu-1}}^{s} \frac{1}{j!} a_{r,j_1}\cdots a_{r,j_\mu} \times \\ & \qquad (F_p^{j_1})^{(\delta_1-1)} \cdots (F_p^{j_\mu})^{(\delta_\mu-1)}\Big|_{h=0} [\psi](p) \qquad (4.10)\end{aligned}$$

for $q = 1, 2, \ldots$. First we set $q = 1$. The only tree in T_O^2 (and S_O^2) is $[\tau]$, so we get

$$\frac{d}{dh}(\psi \circ Y_r)\Big|_{h=0} = \sum_{j=1}^{s} a_{rj}\, (F_p^j)^{(0)}\Big|_{h=0} [\psi](p) = \sum_{j=1}^{s} a_{rj}\mathbb{F}_p([\tau])[\psi](p)$$

for $1 \le r \le s+1$. Moreover $\Phi_r([\tau]) = \sum_{j=1}^{s} a_{r,j}$, $1 \le r \le s+1$, and $\alpha([\tau]) = \gamma([\tau]) = 1$, thus formulas (4.8) and (4.6) hold for $q = 1$.

We proceed by induction: Substitute q by k in (4.8) and (4.9) and assume that the formulas hold for $1 \le k \le q-1$ where $q > 1$ is an arbitrary integer. Note that $q + 1 = 1 + \delta_1 + \cdots + \delta_\mu$ in (4.10), thus each $\delta_\nu - 1 \le q - 1$. We use the induction hypothesis and substitute (4.9) in (4.10) to obtain

$$\begin{aligned}\frac{d^q}{dh^q}(\psi \circ Y_r)\Big|_{h=0} &= \sum_{u\in S_O^{q+1}} \frac{q!}{\prod_{\nu=1}^{\mu}(\delta_\nu - 1)!} \sum_{j_1=1}^{s} \cdots \sum_{j_\mu=j_{\mu-1}}^{s} \frac{1}{j!} a_{r,j_1}\cdots a_{r,j_\mu} \times \\ \sum_{t_1\in T_O^{\delta_1}} \alpha(t_1)\gamma(t_1)\Phi_{j_1}(t_1)\mathbb{F}_p([t_1]) &\cdots \sum_{t_\mu\in T_O^{\delta_\mu}} \alpha(t_\mu)\gamma(t_\mu)\Phi_{j_\mu}(t_\mu)\mathbb{F}_p([t_\mu])[\psi](p) \qquad (4.11)\end{aligned}$$

where $1 \le r \le s+1$.

We now make two observations. First, to each $u \in S_O^{q+1}$ characterized by the ordered tuple $(\delta_1, \ldots, \delta_\mu)$, there is a bijection between $T_O^{\delta_1} \times \cdots \times T_O^{\delta_\mu}$ and the subset of T_O^{q+1} consisting of trees with exactly μ ramifications at the root, namely the one that maps $(t_1,\dots,t_\mu)$ to $t=[t_1,\dots,t_\mu]$. Consequently, we can replace

$$\sum_{u\in S_O^{q+1}}\ \sum_{t_1\in T_O^{\delta_1}}\cdots\sum_{t_\mu\in T_O^{\delta_\mu}} \quad \text{with} \quad \sum_{t\in T_O^{q+1}}.$$

Secondly, all the operators (vector fields) $\mathbb{F}_p([t_i])$ in the above expression have frozen coefficients, hence we find

$$\begin{aligned}\mathbb{F}_p([t_1])\cdots\mathbb{F}_p([t_\mu])[\psi](p) &= \sum_{k_1}\mathbb{F}_p(t_1)[f_{k_1}]E_{k_1}\cdots\sum_{k_\mu}\mathbb{F}_p(t_\mu)[f_{k_\mu}]E_{k_\mu}[\psi](p)\\ &= \sum_{k_1,\dots,k_\mu}\mathbb{F}_p(t_1)[f_{k_1}]\cdots\mathbb{F}_p(t_\mu)[f_{k_\mu}]E_{k_1}\cdots E_{k_\mu}[\psi](p)\\ &= \mathbb{F}_p([t_1,\dots,t_\mu]). \qquad (4.12)\end{aligned}$$

We can now employ (4.12) and Lemma 4.4 to (4.11), keeping in mind that $q=\rho(t)-1$ where $t=[t_1,\dots,t_\mu]$ to obtain the stated formulas (4.8) and (4.6). □

5 Reduction of order conditions

It turns out that several of the conditions in Corollary 4.3 depend on each other, hence only a subset of them needs to be considered. The key observation is the following: Let S_μ be the symmetric group of order μ and for each $i=1,\dots,\mu$, let $\sigma_i=(12\cdots i)\in S_\mu$ written in cyclic notation, i.e.

$$\sigma_i:(p_1,\dots,p_i,p_{i+1},\dots,p_\mu)\mapsto(p_2,\dots,p_i,p_1,p_{i+1},\dots,p_\mu).$$

Let $t_i\in T_O,\ i=1,\dots,\mu$. By a straightforward induction proof, we can establish the identity

$$\Phi([t_1])\Phi([t_2,\dots,t_\mu]) = \sum_{i=1}^{\mu}\Phi([t_{\sigma_i(1)},\dots,t_{\sigma_i(\mu)}]),\quad \mu\ge 2. \qquad (5.1)$$

It is easily verified (again by induction) that (5.1) is consistent with the conditions of Corollary 4.3, i.e.

$$(\gamma([t_1])\gamma([t_2,\dots,t_\mu]))^{-1}=\sum_{i=1}^{\mu}\left(\gamma([t_{\sigma_i(1)},\dots,t_{\sigma_i(\mu)}])\right)^{-1}.$$

Actually, Tracogna and Welfert [15] have shown that (5.1) is a special case of the more general relation

$$\sum_{\substack{\sigma=\sigma_{i_m}\cdots\sigma_{i_1}\\ m\le i_1\le\cdots\le i_m\le\mu}}\Phi([t_{\sigma^{-1}(1)},\dots,t_{\sigma^{-1}(\mu)}])=\Phi([t_1,\dots,t_m])\Phi([t_{m+1},\dots,t_\mu]),$$

$1 \leq m < \mu$. For our purpose it is sufficient to consider (5.1), but the interested reader should consult [15] for the complete solution of the reduction problem.

To make use of the identity (5.1), let $\{t_1, \ldots, t_\mu\} \subset T_O$ be any collection of trees and assume that the coefficients of the Crouch-Grossman method (2.3) are chosen such that

$$\Phi([t_i]) = \frac{1}{\gamma([t_i])}, \qquad i = 1, \ldots, \mu,$$

and

$$\Phi([t_{\sigma(1)}, \ldots, t_{\sigma(\mu-1)}]) = \frac{1}{\gamma([t_{\sigma(1)}, \ldots, t_{\sigma(\mu-1)}])}, \ \forall \sigma \in S_\mu.$$

We now consider the order conditions corresponding to the set of trees

$$J = \left\{ t = [t_{\sigma(1)}, \ldots, t_{\sigma(\mu)}] : \sigma \in S_\mu \right\}.$$

For each permutation $\sigma \in S_\mu$ we obtain a linear equation in the quantities $\{\Phi(t) : t \in J\}$. More precisely, from (5.1) we get

$$\text{(5.2)} \quad \sum_{i=1}^{\mu} \Phi([t_{\sigma_i \sigma(1)}, \ldots, t_{\sigma_i \sigma(\mu)}]) = \frac{1}{\gamma([t_{\sigma(1)}, \ldots, t_{\sigma(\mu-1)}])\gamma([t_{\sigma(\mu)}])}, \ \forall \sigma \in S_\mu.$$

Clearly, of the $\mu!$ linear equations above, some will be identical unless all of $t_1, \ldots, t_\mu$ are distinct. Specifically, if there are ν distinct trees $t_1, \ldots, t_\nu$ and the tree t_i appears ℓ_i times there will be a total of

$$n_\ell := \frac{\mu!}{\ell_1! \cdot \ell_2! \cdots \ell_\nu!}$$

distinct linear equations in (5.2). In any case, given the set $\{t_1, \ldots, t_\mu\}$, (5.2) defines a linear transformation $L : \mathbb{R}^{n_\ell} \to \mathbb{R}^{n_\ell}$. It is then possible to partition the set J into subsets J_1 and J_2 and express each $\Phi(t)$, $t \in J_1$, in terms of the elements of the set $\{\Phi(t) : t \in J_2\}$. Then J_1 has precisely rank L elements and J_2 has $\dim(\ker L)$ elements. In conclusion, it is at most necessary to consider $N_L := \dim(\ker L)$ order conditions from the set J. Note that if there are ν distinct trees among $t_1, \ldots, t_\mu$, and the ith of these distinct trees occurs ℓ_i times, N_L depends only on $\ell_1, \ldots, \ell_\nu$, i.e. $N_L = N_L(\ell_1, \ldots, \ell_\nu)$. The precise expression for N_L can be found in another paper by Tracogna and Welfert [16].

For the single tree generated by $\mu \geq 2$ copies of the tree t_1, i.e. $t = [t_1, \ldots, t_1]$, we clearly have $N_L(\mu) = 0$, thus the order condition corresponding to t is satisfied if $\Phi([t_1]) = 1/\gamma([t_1])$.

Next we consider the case with $\mu - 1$ copies of the tree t_1 and one occurrence of a different tree t_2. The corresponding set of trees J has μ elements. By a natural choice of basis for the linear transformation above, we obtain the matrix representation $\hat{L}$ of L

$$\hat{L} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ \mu - 1 & 1 & 0 & \cdots & 0 \\ 0 & \mu - 2 & 2 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & \mu - 1 \end{bmatrix}.$$

Clearly rank $\hat{L} = \mu - 1$, the first row multiplied by $\mu - 1$ equals the sum of the remaining rows. Any choice of $\mu - 1$ columns of $\hat{L}$ results in a linearly independent set. In conclusion: It is sufficient to include one of the μ order conditions corresponding to the set J, and the choice of order condition is arbitrary.

These observations can be used to find the minimal number of order conditions that must be satisfied by methods with $q \leq 5$. For methods of higher order one must use the theory of [15] to determine the minimal number of conditions that must be considered.

We illustrate the above discussion by applying the results to the order conditions up to order 4, conditions corresponding to trees with $q + 1$ nodes, $q = 1, \ldots, 4$. Referring to Table 4.1 we recognize the trees $t_{31}, t_{41}, t_{501}, t_{509}$ as being of the form $[t, t, \ldots, t]$ with at least two occurrences of t in the bracket.

Furthermore from each of the sets $\{t_{42}, t_{43}\}$, $\{t_{501}, t_{502}, t_{503}\}$, $\{t_{505}, t_{506}\}$, and $\{t_{507}, t_{508}\}$ we need only consider the order condition corresponding to *one* (arbitrary) member.

In conclusion, a sufficient selection of order conditions to be satisfied are those corresponding to the following trees.

Order 1.

$$t_{21}: \qquad \sum_{r=1}^{s} b_r = 1$$

Order 2.

$$t_{32}: \qquad \sum_{r=1}^{s} b_r \, c_r = \frac{1}{2}$$

Note that the conditions for orders 1 and 2 are exactly the same as for standard Runge-Kutta methods, thus, by choosing the coefficients of any such method with (classical) order ≥ 2 we obtain at least order 2 also in the Crouch-Grossman case.

Order 3.

$$t_{42}: \quad \sum_{r=1}^{s} b_r\, c_r \left(\frac{1}{2} b_r + \sum_{j=r+1}^{s} b_j \right) = \frac{1}{6}$$

$$t_{44}: \quad \sum_{r=1}^{s} \sum_{j=1}^{s} b_r a_{rj} c_j = \frac{1}{6}$$

$$t_{45}: \quad \sum_{r=1}^{s} b_r\, c_r^2 = \frac{1}{3}$$

Note that the only extra condition compared to the standard case stems from t_{42}. This condition is nonlinear in the b_r-coefficients and it can also be found in [3] for explicit methods with three stages.

Order 4. A sufficient set is $\{t_{502}, t_{505}, t_{507}, t_{510}, t_{511}, t_{512}, t_{513}, t_{514}\}$. We write out only those of the conditions that differ from the standard case.

$$t_{502}: \quad \sum_{r=1}^{s} b_r\, c_r \left(\frac{1}{6} b_r^2 + \sum_{j=r+1}^{s} b_j \left(\frac{1}{2} b_r + \frac{1}{2} b_j + \sum_{k=j+1}^{s} b_k \right) \right) = \frac{1}{24}$$

$$t_{505}: \quad \frac{1}{2} \sum_{r=1}^{s} b_r\, c_r^2 \left(\frac{1}{2} b_r + \sum_{j=r+1}^{s} b_j \right) = \frac{1}{24}$$

$$t_{507}: \quad \sum_{r=1}^{s} \sum_{j=1}^{s} b_r a_{rj} c_j \left(\frac{1}{2} b_r + \sum_{k=r+1}^{s} b_k \right) = \frac{1}{24}$$

$$t_{511}: \quad \sum_{r=1}^{s} \sum_{j=1}^{s} b_r a_{rj} c_j \left(\frac{1}{2} a_{rj} + \sum_{k=j+1}^{s} a_{rk} \right) = \frac{1}{24}$$

$$t_{512}: \quad \sum_{r=1}^{s} \sum_{j=1}^{s} b_r a_{rj} \left(\frac{1}{2} a_{rj} c_j + \sum_{k=j+1}^{s} a_{rk} c_k \right) = \frac{1}{8}$$

Note that if one adds up the conditions corresponding to t_{511} and t_{512} one obtains the classical order condition corresponding to the (non-ordered) tree $[\tau, [\tau]]$, see also Remark 4.2.

6 Examples of methods

6.1 Explicit methods

Explicit methods of order three have already been developed by Crouch and Grossman [3]. We give one example method with three stages in the Butcher tableau below.

$$
\begin{array}{c|ccc}
0 & 0 & & \\
\frac{3}{4} & \frac{3}{4} & & \\
\frac{17}{24} & \frac{119}{216} & \frac{17}{108} & \\
\hline
 & \frac{13}{51} & -\frac{2}{3} & \frac{24}{17}
\end{array}
\tag{6.1}
$$

For methods of order 4 there are a total of 13 order conditions versus 8 in the standard case. The search for solutions of the order conditions is further complicated by the nonlinearity in the b_r-coefficients. By careful investigation of the order conditions, we found that it is not possible to obtain explicit methods of order 4 with only 4 stages. The proof is technical and is not included here. We therefore tried to find methods with 5 stages. To reduce the complexity in the conditions, we introduced simplifying assumptions, requiring that

$$\sum_{j=1}^{s} a_{rj} c_j = \frac{1}{2} c_r^2, \quad \forall\ r \neq 2.$$

Under these assumptions we found certain solutions, an example is

$$
\begin{array}{ll}
c_2 = \frac{3}{2} & c_3 = \frac{1}{3}\kappa + \frac{1}{6}\kappa^2 + \frac{2}{3} \\
c_4 = -\frac{1}{3}\kappa - \frac{1}{6}\kappa^2 + \frac{1}{3} & c_5 = 1 \\
b_1 = b_5 = \dfrac{1}{2} \cdot \dfrac{1+\kappa+\kappa^2}{\kappa+\kappa^2} & b_2 = 0 \\
b_3 = -\dfrac{1}{6} \cdot \dfrac{1+2\kappa+\kappa^2}{2+\kappa+\kappa^2} & b_4 = -\dfrac{1}{2} \cdot \dfrac{1}{\kappa+\kappa^2} \\
a_{32} = \frac{1}{18}(4+3\kappa+2\kappa^2) & a_{42} = (1+\kappa+\kappa^2)\theta - \frac{1}{18}(4+3\kappa+2\kappa^2) \\
a_{52} = \theta & a_{43} = \dfrac{-9(1+\kappa+\kappa^2)\theta + 3 + \kappa + \kappa^2}{4+2\kappa+\kappa^2} \\
a_{54} = -\dfrac{\kappa+\kappa^2}{4+2\kappa+\kappa^2} & a_{53} = \dfrac{-9(1+\kappa+\kappa^2)\theta + 3 + 2\kappa + 2\kappa^2}{10+8\kappa+7\kappa^2}.
\end{array}
\tag{6.2}
$$

where $\kappa = 2^{1/3}$ and θ is a root of the quadratic equation

$$81\theta^2 - 9(1+\kappa+\kappa^2)\theta - (25+21\kappa+17\kappa^2) = 0.$$

6.2 SDIRK and ESDIRK methods

An SDIRK method with three stages can be represented in the following Butcher tableau (see e.g. [6])

$$
(6.3)\qquad
\begin{array}{c|ccc}
\gamma & \gamma & & \\
c_2 & a_{21} & \gamma & \\
c_3 & a_{31} & a_{32} & \gamma \\
\hline
 & b_1 & b_2 & b_3
\end{array}
\qquad\qquad
\begin{array}{c|ccc}
1 & 1 & & \\
\frac{5}{8} & -\frac{3}{8} & 1 & \\
\frac{23}{48} & -\frac{125}{432} & -\frac{25}{108} & 1 \\
\hline
 & \frac{31}{75} & -\frac{4}{3} & \frac{48}{25}
\end{array}
$$

It is not clear to us what the desired properties of a Crouch-Grossman type of SDIRK method should be, for an example, we derived a method of order 3 which is A-stable (but not L-stable) in the standard case given to the right above.

Recently, Kværnø [8] has derived improved candidates among a type of methods, denoted ESDIRK methods. These seem to have better properties than the SDIRK methods for classical problems. The methods are stiffly accurate and use an explicit first stage, thereby acquiring the FSAL property, hence they effectively cost one less stage per step. With 4 (effectively 3) stages, the methods are of the form

$$
(6.4)\qquad
\begin{array}{c|cccc}
0 & 0 & & & \\
c_2 & a_{21} & \gamma & & \\
c_3 & a_{31} & a_{32} & \gamma & \\
1 & b_1 & b_2 & b_3 & \gamma \\
\hline
 & b_1 & b_2 & b_3 & \gamma
\end{array}
\qquad\qquad
\begin{array}{c|cccc}
0 & 0 & & & \\
\frac{3}{4} & -\frac{1}{4} & 1 & & \\
\frac{25}{24} & \frac{59}{216} & -\frac{25}{108} & 1 & \\
1 & \frac{22}{75} & \frac{2}{3} & -\frac{24}{25} & 1 \\
\hline
 & \frac{22}{75} & \frac{2}{3} & -\frac{24}{25} & 1
\end{array}
$$

An A-stable (but not L-stable) example of such a Crouch-Grossman method of order 3 with rational coefficients is given to the right. It turns out that the extra order condition corresponding to t_{42} of Table 4.1 can be fulfilled without making any major restrictions on the parameter γ. By choosing $\gamma \approx 0.43$ one can obtain a method which is L-stable in the classical sense.

7 Application to Lie groups

A *Lie group* G is a differentiable manifold equipped with a group structure such that the map

$$
\begin{array}{rcl}
G \times G & \to & G \\
(y, z) & \mapsto & y \cdot z^{-1}, \quad y, z \in G,
\end{array}
$$

is smooth. By using this group operation, we define a diffeomorphism of G by means of *right multiplication*, i.e. for any $y \in G$, let $R_y : G \to G$ be the map

$$R_y(z) = z \cdot y, \quad \forall z \in G.$$

There is an identity element in G, henceforth denoted e. The tangent space at e, $\mathfrak{g} := TG_e$, equipped with a bilinear, skew-symmetric operation denoted the *Lie bracket*, $[\cdot,\cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, is called the *Lie algebra* of G. This operation can be defined as follows: For any $v \in \mathfrak{g}$ let X_v be the *right invariant vector field*

$$X_v : y \mapsto dR_y(v).$$

The set of right invariant vector fields is isomorphic to $\mathfrak{g}$. Let Z be the operator

$$Z = X_v \circ X_w - X_w \circ X_v.$$

It can then be shown (see e.g. [18]) that Z is a smooth right invariant vector field, hence there is an element $u \in \mathfrak{g}$ such that $Z = X_u$. We define the bracket $[v,w] := u$.

The map $dR_y : \mathfrak{g} \to TG_y$ is an isomorphism of the tangent spaces TG_e and TG_y. Therefore, any smooth vector field on G can be written in the form

$$F : y \mapsto dR_y(f(y)), \quad f : G \to \mathfrak{g}. \tag{7.1}$$

Let $v_1, \ldots, v_n$ be a basis for $\mathfrak{g}$. We may now choose the frame vector fields E_i as right invariant vector fields

$$E_i : y \mapsto dR_y(v_i), \quad i = 1, \ldots, n,$$

and it follows that $f(y) = \sum_{i=1}^n f_i(y) v_i$ with $f_i(y)$ defined by (2.1).

In the case that G is a *matrix Lie group* (see e.g. [5]) the Crouch-Grossman methods take a particularly simple form through the use of the matrix exponential. The group elements are now invertible $m \times m$-matrices, and we associate each element in the Lie algebra with an $m \times m$-matrix v such that the matrix exponential $e^v \in G$. The Lie bracket is simply the *matrix commutator* $[v,w] = v \cdot w - w \cdot v$ and the flow of a vector field $X_v \in \mathcal{V}$ can be computed with the formula

$$e^{tX_v} y = e^{tv} \cdot y,$$

where the matrix exponential is used on the right hand side. A consequence of this is that the flows occurring in the Crouch-Grossman methods (2.3) are obtained by computing the matrix exponential of the function $f(y)$ occurring in (7.1) for various values of y.

Examples of Lie matrix groups and their Lie algebras are

1. The *general linear group* $GL(m)$, consisting of all invertible $m \times m$ matrices. The corresponding Lie algebra is $\mathfrak{gl}(m)$ the vector space of all $m \times m$ matrices.

2. The group of $m \times m$ orthogonal matrices with determinant 1, denoted $SO(m)$. This is a connected subgroup of $GL(m)$. The Lie algebra is $\mathfrak{so}(m)$, the vector space of skew-symmetric $m \times m$ matrices and its dimension is $m(m-1)/2$.

Any vector space V (not necessarily of matrices) has the structure of an abelian Lie group where the binary operation is addition, $v^{-1} = (-v)$ for each $v \in V$, and the identity element e is the zero vector. The Lie algebra is isomorphic to V itself and the Lie bracket $[x, y] = 0$ for all $x, y \in V$.

The cartesian product $G_1 \times G_2$ between two Lie groups G_1 and G_2 can again be made into a Lie group through the multiplication rule

$$(\sigma_1, \sigma_2) \cdot (\tau_1, \tau_2) = (\sigma_1 \cdot \tau_1, \sigma_2 \cdot \tau_2), \quad \sigma_1, \tau_1 \in G_1,\ \sigma_2, \tau_2 \in G_2.$$

If $\mathfrak{g}_1$ and $\mathfrak{g}_2$ are the Lie algebras of G_1 and G_2 respectively, then $\mathfrak{g}_1 \times \mathfrak{g}_2$ is the Lie algebra of $G_1 \times G_2$.

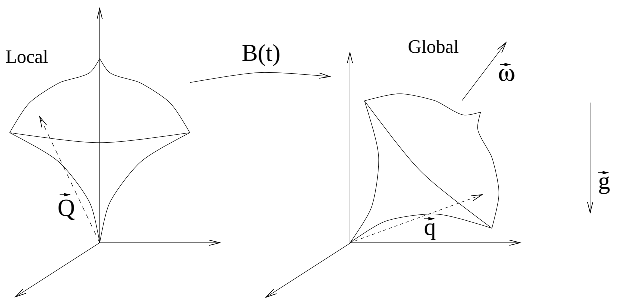

Figure 7.1: A schematic picture of the spinning top in local and global coordinates.

Example. We shall apply our theory to *the spinning top* in Figure 7.1, see e.g. [1, 9]. The top is modeled as a rigid body, suspended at one point. Its position can be represented as a rotation which transforms a point in local coordinates to global coordinates. Such a rotation $B = B(t)$ can be represented as an element of the Lie group $SO(3)$, the group of orthogonal 3×3-matrices with determinant one. The tangent to $B(t)$ is $\dot{B}(t) \in TSO(3)_{B(t)}$ and can therefore be written in the form $\dot{B}(t) = \omega(t) \cdot B(t)$, where $\omega(t) \in \mathfrak{so}(3)$. We call $\omega(t)$ the *angular momentum* of the spinning top. From a physical perspective it is natural to think of $\omega(t)$ as a 3-vector $\vec{\omega}(t)$ defined by the identification

$$\vec{\omega} = \begin{bmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \end{bmatrix} \leftrightarrow \begin{bmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{bmatrix} = \omega.$$

The configuration of the spinning top can be described by the pair

$$\big(B(t), \omega(t)\big) \in SO(3) \times \mathfrak{so}(3) =: G.$$

Thus, G is a cartesian product of two Lie groups. The Lie algebra can be identified with $\mathfrak{g} := \mathfrak{so}(3) \times \mathfrak{so}(3)$. We list some properties of this Lie group/algebra:

Product in G:	$(a, v) \cdot (b, w) = (a \cdot b, v + w)$.
Addition in $\mathfrak{g}$:	$(u, v) + (\widetilde{u}, \widetilde{v}) = (u + \widetilde{u}, v + \widetilde{v})$.
Multiplication by scalar in $\mathfrak{g}$:	$\alpha(u, v) = (\alpha u, \alpha v)$.
Lie bracket in $\mathfrak{g}$:	$[(u, v), (\widetilde{u}, \widetilde{v})] = ([u, \widetilde{u}], 0)$.
Exponential map from $\mathfrak{g}$ to G:	$\exp(u, v) = (\exp(u), v)$.

The dynamics of the spinning top is discussed in many text books, see for instance [1]. Denote by $\vec{g}$ the external forces, e.g. gravitation, let A be the inertia tensor, and $\vec{C}$ the center of mass of the spinning top. Define

$$\begin{aligned} f \quad &: \quad G \to \mathfrak{g} \\ &\quad (r, \omega) \mapsto (\omega, \omega'), \end{aligned}$$

where

$$\vec{\omega}' = -BA^{-1}B^T \, \omega \, BAB^T \, \vec{\omega} + BA^{-1}B^T \, (B\vec{C} \times \vec{g}).$$

We obtain the differential equation

$$\frac{d}{dt}(B(t), \omega(t)) = dR_{(B(t),\omega(t))} \left(f(B(t), \omega(t)) \right).$$

If we write out the right hand side in terms of matrix products we get

$$dR_{(B,\omega)} \left(f(B, \omega) \right) = (\omega \cdot B, \omega').$$

The flows of vector fields appearing in (2.3) are now computed using the exponential map defined above for suitable values of the function $f : G \to \mathfrak{g}$.

We have implemented the schemes CG3 (6.1), CG4 (6.2), SDIRK3 (6.3) and ESDIRK3 (6.4) in MATLAB and applied them to the spinning top test problem, the main purpose being to verify the order theory presented in this paper. The initial data of the simulations were

$$B_0 = \begin{bmatrix} 1.0 & 0.0 & 0.0 \\ 0.0 & \cos(\phi) & \sin(\phi) \\ 0.0 & -\sin(\phi) & \cos(\phi) \end{bmatrix} \quad \text{and} \quad \omega_0 = \begin{bmatrix} 0.0 & -1.0 & 0.0 \\ 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 \end{bmatrix}$$

with $\phi = \pi/16$. The inertia tensor, the center of mass and the external forces were given as

$$A = \frac{1}{8} \begin{bmatrix} 7 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \qquad \vec{C} = \begin{bmatrix} 0 \\ 0 \\ \sqrt{3}/2 \end{bmatrix}, \qquad \text{and} \qquad \vec{g} = \begin{bmatrix} 0 \\ 0 \\ -9.81 \end{bmatrix}.$$

Figure 7.2 shows the global error versus stepsize of CG3 and CG4. For comparison, we implemented "the Runge-Kutta method", RK4 [6, p. 138], using the format (2.3). The lines in the plot are included for reference, they have slopes 2, 3 and 4. Note that even though RK4 has order 4 in the classical sense, it

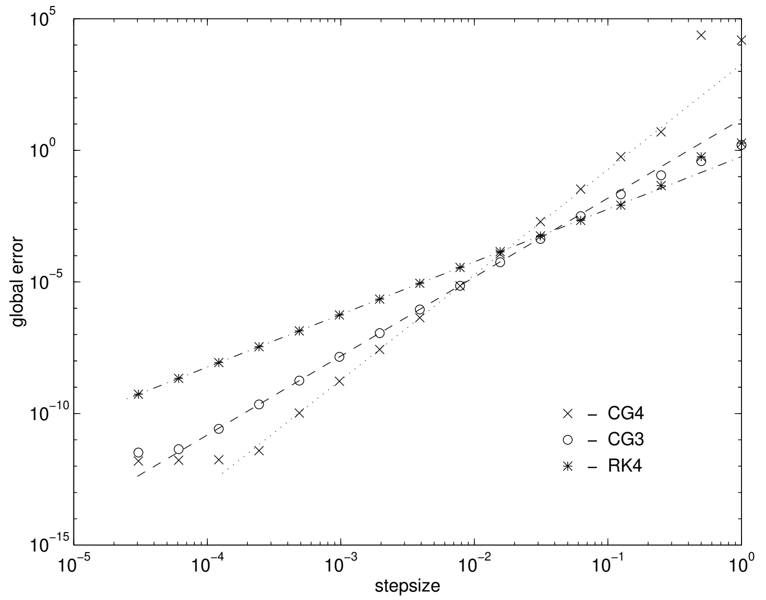

Figure 7.2: Global error versus stepsize for the schemes CG3, CG4 and RK4

exhibits only order 2 in the Crouch-Grossman setting. This is consistent with the fact that additional order conditions are introduced only from order 3.

The same type of data is plotted in Figure 7.3 for the SDIRK3 and ESDIRK3 methods. The straight line has slope 3. The non-linear equations are solved in each step by means of the Newton iteration on Lie groups as presented in [14], iterating to machine accuracy for each stage. The experiments show that for the spinning top problem, implicit methods are very inefficient, but the tests still serve their purpose here.

In all the experiments, the global error was computed by first applying the MATLAB library routine `ODE45` with tolerance 10^{-14}. The error was measured using the sum of the 2-norm of each solution component.

We remark that the above explicit methods applied to the spinning top problem are examples of *explicit orthogonal integrators*, see [7] for a discussion of orthogonal integrators. It is known that classical methods cannot both be explicit and preserve orthogonality. However, it is known that for instance the classical Gauss methods do preserve orthogonality. This fact may also indicate that the implicit Crouch-Grossman method is a poor choice for this type of problems. To demonstrate the preservation of orthogonality in the explicit Crouch-Grossman method, we have plotted in Figure 7.4 the quantity $\|B(t)^T B(t) - B(0)^T B(0)\|_2$ as a function of time for the method CG3 and for RK4 implemented in the classical way. For the approximations obtained with CG3, the drift from the manifold $SO(3)$ is of a magnitude consistent with the machine accuracy.

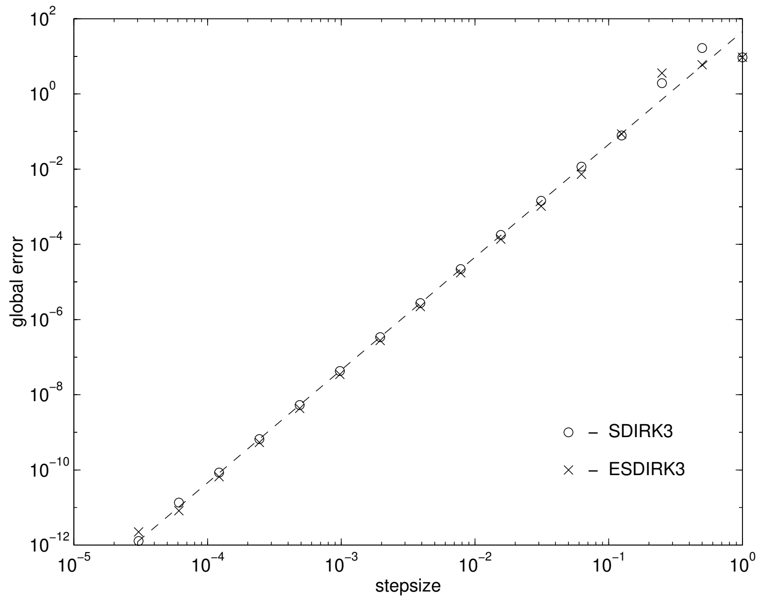

Figure 7.3: Global error versus stepsize for the schemes SDIRK3 and ESDIRK3

8 Concluding remarks

We have presented a type of method which is a generalization of Runge-Kutta methods. Rather than being able to move only along straight lines in a vector space, the primitives of the Crouch-Grossman methods consist of flows belonging to the linear span of certain frame vector fields that can be chosen at liberty by the user to accommodate any particular application. It is thus assumed that the user has the means to evaluate or approximate these flows, and the theory does not consider the effect of any inaccuracies in the computation of these flows. It is not clear how the frame vector fields should be chosen in general. For certain types of manifolds, there will be a natural choice of frame vector fields, for instance, for Lie groups one will typically choose a basis for the corresponding Lie algebra. If the Lie group is a matrix group, the evaluation of a flow will amount to the computation of a matrix exponential. In certain applications this can be done cheaply, for instance if the group consists of rotations in 3D, one can make use of the Rodrigues formula [5] for this purpose. In the general case, the computation of matrix exponentials may be time consuming.

As for classical Runge-Kutta methods, implementation issues include error control and stepsize variation strategies. It it natural to look for embedded pairs of method coefficients. This, however, requires a metric on the manifold, typically realized by using a specific coordinate system.

It seems that the type of method presented here is only one of many possible generalizations of Runge-Kutta methods. A few other approaches have been

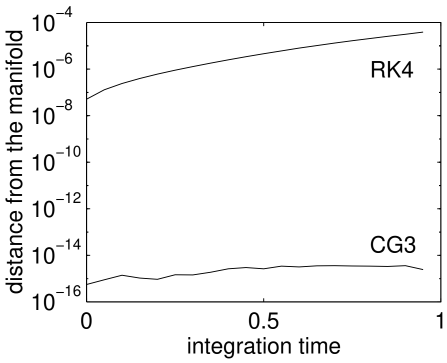

Figure 7.4: $||B(t)^T B(t) - B(0)^T B(0)||_2$ for CG3 and RK4 implemented in the classical way.

proposed by Munthe–Kaas [10, 11]. They differ from the Crouch-Grossman methods in the sense that the coupling between internal stages is performed on vector fields rather than on their flows. Generally the two approaches are not equivalent. We believe that there may be other feasible approaches, not yet discovered, but perhaps the analysis of similar techniques can be done in a similar way to the one presented here. The order conditions derived here are general in the sense that they do not depend on the choice of frame vector fields. We believe that such a criterion may be too restrictive, since our intention is not to design more general schemes, but rather to accommodate integration methods for particular manifolds found in applications. Therefore, it would be important to answer the question of whether the set of order conditions can be reduced for particular choices of manifolds and frame vector fields and thereby obtain less expensive schemes tailored for a particular type of application. For instance, in many problems in structural dynamics, the configuration manifold consists of semidirect products [17, 13] between the rotation group and translations in $\mathbb{R}^3$.

One of the benefits of these new approaches for numerical integration on manifolds is their suitability for object-oriented implementations. For instance, in the definition of the methods, no explicit reference is made to coordinates or to the particular representation of objects like flows or vector fields.

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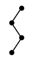
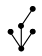
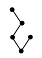
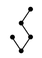
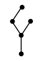
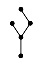
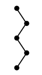
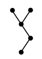
lbl	t	$\gamma(t)$	$\alpha(t)$	$\Phi(t)$
τ	$\bullet$	1	1	1
t_{21}		1	1	$\sum_{r=1}^{s} b_r$
t_{31}		2	1	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} = \frac{1}{2}(\sum_{r=1}^{s} b_r)^2$
t_{32}		2	1	$\sum_{r=1}^{s} b_r c_r$
t_{41}		6	1	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \sum_{r_3=r_2}^{s} \frac{1}{r!} b_{r_1} b_{r_2} b_{r_3} = \frac{1}{6}(\sum_{r=1}^{s} b_r)^3$
t_{42}		6	1	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} c_{r_1}$
t_{43}		3	2	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} c_{r_2}$
t_{44}		6	1	$\sum_{r=1}^{s} \sum_{j=1}^{s} b_r a_{rj} c_j$
t_{45}		6	1	$\sum_{r=1}^{s} b_r \frac{1}{2} c_r^2$
t_{501}		24	1	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \sum_{r_3=r_2}^{s} \sum_{r_4=r_3}^{s} \frac{1}{r!} b_{r_1} b_{r_2} b_{r_3} b_{r_4} = \frac{1}{24}(\sum_{r=1}^{s} b_r)^4$
t_{502}		24	1	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \sum_{r_3=r_2}^{s} \frac{1}{r!} b_{r_1} b_{r_2} b_{r_3} c_{r_1}$
t_{503}		12	2	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \sum_{r_3=r_2}^{s} \frac{1}{r!} b_{r_1} b_{r_2} b_{r_3} c_{r_2}$
t_{504}		8	3	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \sum_{r_3=r_2}^{s} \frac{1}{r!} b_{r_1} b_{r_2} b_{r_3} c_{r_3}$
t_{505}		24	1	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} \frac{1}{2} c_{r_1}^2$
t_{506}		8	3	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} \frac{1}{2} c_{r_2}^2$
t_{507}		24	1	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \sum_{j=1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} a_{r_1 j} c_j$
t_{508}		8	3	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \sum_{j=1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} a_{r_2 j} c_j$
t_{509}		8	3	$\sum_{r_1=1}^{s} \sum_{r_2=r_1}^{s} \frac{1}{r!} b_{r_1} b_{r_2} c_{r_1} c_{r_2} = \frac{1}{2}(\sum_{r=1}^{s} b_r c_r)^2$
t_{510}		24	1	$\sum_{r=1}^{s} b_r \frac{1}{6} c_r^3$
t_{511}		24	1	$\sum_{r=1}^{s} \sum_{j_1=1}^{s} \sum_{j_2=j_1}^{s} \frac{1}{j!} b_r a_{r j_1} a_{r j_2} c_{j_1}$
t_{512}		12	2	$\sum_{r=1}^{s} \sum_{j_1=1}^{s} \sum_{j_2=j_1}^{s} \frac{1}{j!} b_r a_{r j_1} a_{r j_2} c_{j_2}$
t_{513}		24	1	$\sum_{r=1}^{s} \sum_{j=1}^{s} \sum_{k=1}^{s} b_r a_{rj} a_{jk} c_k$
t_{514}		24	1	$\sum_{r=1}^{s} \sum_{j=1}^{s} b_r a_{rj} \frac{1}{2} c_j^2$

Table 4.1: Trees of order ≤ 5 and some associated functions