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2006 J. Phys. A: Math. Gen. 39 5585

(http://iopscience.iop.org/0305-4470/39/19/S15)

Institute of Physics Publishing Journal of Physics A: Mathematical and General
J. Phys. A: Math. Gen. **39** (2006) 5585–5599 doi:10.1088/0305-4470/39/19/S15

Order conditions for commutator-free Lie group methods

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Received 19 December 2005, in final form 27 January 2006
Published 24 April 2006
Online at stacks.iop.org/JPhysA/39/5585

Abstract
We derive order conditions for commutator-free Lie group integrators. For certain problems, these schemes can be good alternatives to the Runge–Kutta–Munthe-Kaas schemes, especially when applied to stiff problems or to homogeneous manifolds with large isotropy groups. The order conditions correspond to certain subsets of the set of ordered rooted trees. We discuss ways to select these subsets and their combinatorial properties. We also suggest how the reuse of flow calculations can be included in order to reduce the computational cost. In the case that at most two flow calculations are admitted in each stage, the order conditions simplify substantially. We derive families of fourth-order schemes which effectively use only five flow calculations per step.

PACS numbers: 02.20.Tw, 02.60.Jh

1. Introduction

Crouch and Grossman [7] were perhaps the first to propose a method format in the general class of integrators which are today recognized as Lie group integrators for solving ordinary differential equations on manifolds. Also Lewis and Simo, see e.g. [13, 14], made significant early contributions to this class. Going even further back, one finds the class of schemes known today as exponential integrators, perhaps first proposed by Certaine [4], an extensive review is given in [16]. Some exponential integrators can be recognized as Lie group integrators with respect to a particular choice of group action. For a complete discussion of the connection between exponential integrators and Lie group integrators, see [12, 15]. See also [9] for stiff order conditions for exponential integrators. More recently the methods known as the Runge–Kutta Munthe-Kaas methods have been developed [17, 18], see also the survey article [11] and the references therein.

Given a differentiable manifold $\mathcal{M}$, we consider the initial value problem

$$\dot{y} = F(y), \qquad y(0) = p \in \mathcal{M}, \tag{1}$$

where $y(t) \in \mathcal{M}$, and $F \in \mathfrak{X}(\mathcal{M})$ is the space of smooth vector fields on $\mathcal{M}$. We shall use *frames* for expressing the numerical integrators: however, one can alternatively use Lie group actions [18]. A frame is here defined as a set of d smooth vector fields, $E_1, \ldots, E_d$ where $d \geqslant m = \dim \mathcal{M}$ and such that for every point $y \in \mathcal{M}$ we have

$$\operatorname{span}\{E_1(y), \ldots, E_d(y)\} = T_y\mathcal{M}. \tag{2}$$

This property plays a similar role to transitivity when schemes are expressed in terms of Lie group actions. In the way we are going to use frames in the following, it is only the linear span $\mathcal{V}$ of the vector fields $E_1, \ldots, E_d$ which matters; in fact, one may assume, without loss of generality, that $E_1, \ldots, E_d$ are linearly independent as vector fields, and thus constitute a basis for $\mathcal{V}$. A change of basis for $\mathcal{V}$ is not going to affect the approximation obtained from the integration scheme.

As an example of a linear space $\mathcal{V}_A$ of vector fields on $\mathbf{R}^m$, with $m = d - 1$ one may consider, for a fixed matrix $L \in \mathbf{R}^{m\times m}$

$$\mathcal{V}_A = \{F : F(y) = \alpha L y + b, \alpha \in \mathbf{R}, b \in \mathbf{R}^m\} \tag{3}$$

which is the choice underlying the exponential integrators.

The property (2) allows us to write an arbitrary smooth vector field F as in (1) in the form

$$F(y) = \sum_{i=1}^{d} f_i(y) E_i(y), \tag{4}$$

for some functions $f_i \in C^\infty(\mathcal{M}, \mathbf{R})$. As usual, we define the *flow* of a vector field F to be the one-parameter family of diffeomorphisms $\exp(tF)$ defined on some t-dependent subset of $\mathcal{M}$ such that $\exp(tF)p$ is the solution $y(t)$ of (1) with initial value $y(0) = p$.

The notion of a *frozen vector field* is important when Lie group integrators are formulated in terms of frames. Given a vector field F in the form (4) and a point $p \in \mathcal{M}$, we associate a vector field $F_p \in \mathcal{V}$ defined as

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

The schemes of Crouch and Grossman [7] are designed by composing flows of vector fields frozen at various points near the initial value of the step. Recently Celledoni *et al* [3] proposed a new type of schemes which include the Crouch–Grossman class as a special case.

$$\left.\begin{aligned} g_r &= \exp\left(\sum_k \alpha_{r,J}^k F_k\right) \cdots \exp\left(\sum_k \alpha_{r,1}^k F_k\right)(p) \\ F_r &= h F_{g_r} = h \sum_i f_i(g_r) E_i, \end{aligned}\right\}, \qquad r = 1, \ldots, s, \tag{5}$$
$$y_1 = \exp\left(\sum_k \beta_J^k F_k\right) \cdots \exp\left(\sum_k \beta_1^k F_k\right) p.$$

The coefficients of the methods are $\left(\alpha_{r,j}^k\right)$, $1 \leqslant r, k \leqslant s$, $1 \leqslant j \leqslant J$ and $\left(\beta_j^k\right)$, $1 \leqslant k \leqslant s$, $1 \leqslant j \leqslant J$. We note that scheme (5) is explicit if $\alpha_{r,j}^k = 0$ whenever $k \geqslant r$. The motivation for proposing this new scheme is twofold. On the one hand, there are problems in which the use of commutators may be undesirable, for instance in the solution of stiff systems or on homogeneous spaces with large isotropy groups, see [3]. On the other hand, the schemes of Crouch and Grossman, which avoid the use of commutators, involve a very large number of flow computations (exponentials). For instance, in an s stage explicit Crouch–Grossman method, there will be as many as $s(s+1)/2$ exponentials to compute in each step. The main idea behind these new schemes is to choose the number J of exponentials per stage as low as possible; clearly, one may use a different J for each stage.

We shall adopt the definition from [20] of order of consistency (or simply order) of an integration scheme, by saying that a scheme, represented as a map $\chi_h : \mathcal{M} \to \mathcal{M}$, has order q if for any smooth function $\psi \in C^\infty(\mathcal{M}, \mathbf{R})$ and point $p \in \mathcal{M}$ one has

$$\psi(\exp(hF)p) - \psi(\chi_h(p)) = \mathcal{O}(h^{q+1}) \qquad \text{as } h \to 0. \tag{6}$$

The conditions one needs to impose on the coefficients of scheme (5) such that (6) holds for some prescribed q, will be called *order conditions*.

In this paper we will derive a complete set of order conditions for methods of format (5). In section 2, we extend the results of [20] where order conditions were derived for the schemes of Crouch and Grossman [7]. In section 2.4, we shall see how the conditions can be significantly simplified in the case that $J = 2$ in (5). Then, in section 4, we provide examples of schemes, and we will show how reuse of exponentials can reduce the computational cost of the schemes.

2. Order conditions in terms of rooted ordered trees

The schemes (5) are defined for an arbitrary choice of frame, in particular one can choose $\mathcal{M}$ to be a Euclidean space with global coordinate system $(x_1, \ldots, x_d)$, and the vector fields $E_i = \frac{\partial}{\partial x_i}$. The flow of an element in the span of these vector fields is just translation, $\exp(tV)p = p + tV$, where $V = \sum_i V_i \frac{\partial}{\partial x_i}$. With this choice of frame, it follows that the scheme (5) reduces to a classical Runge–Kutta scheme

$$\left.\begin{aligned} g_r &= p + \sum_k a_r^k F_k \\ F_r &= hF_{g_r} \end{aligned}\right\}, \qquad r = 1, \ldots, s,$$

$$y_1 = p + \sum_r b^r F_r,$$

where $a_r^k = \sum_j \alpha_{r,j}^k$ and $b^r = \sum_j \beta_j^r$. So, a necessary condition for the scheme to have order p for a general frame, is that the coefficients a_r^k, b^k defined above, satisfy the classical order conditions for Runge–Kutta methods.

2.1. Trees and elementary differentials

For studying the schemes proposed above, we shall use a generalization of Butcher series [2, 8] based on the use of rooted trees. In the classical order theory for Runge–Kutta methods, the trees are non-ordered trees, meaning that no ordering is imposed on the set of subtrees of a tree. However, as explained in [20], we here need to use ordered rooted trees. We denote by T_O the set of all ordered rooted trees. A tree $t \in T_O$ if either $t = \bullet$, or if $t = B_+(t_1, \ldots, t_\mu)$ with each $t_i \in T_O$. B_+ maps an ordered set of trees in T_O to one tree in T_O by connecting the root of each tree t_i to a new common root. Similarly we define the map B_- which assigns to a tree in T_O the (ordered) set of its subtrees. In particular, we set $B_+(\emptyset) = \bullet$ and $B_-(\bullet) = \emptyset$. The number of nodes in the tree is denoted as $|t|$, so we have $|\bullet| = 1$ and for $t = B_+(t_1, \ldots, t_\mu)$ we have $|t| = 1 + \sum_i |t_i|$. We define a non-commutative concatenation product between elements in T_O. The tree $\bullet$ is the unit element, i.e. $\bullet \cdot t = t \cdot \bullet = t$ for every $t \in T_O$. For trees $u = B_+(u_1, \ldots, u_\mu)$ and $v = B_+(v_1, \ldots, v_\nu)$, we set $u \cdot v = B_+(B_-(u), B_-(v)) = B_+(u_1, \ldots, u_\mu, v_1, \ldots, v_\nu)$. Note that $|u \cdot v| = |u| + |v| - 1$.

We can now generalize the concept of elementary differentials by associating with each tree $t \in T_O$ a differential operator $\mathbf{F}(t) : C^\infty(\mathcal{M}, \mathbf{R}) \to C^\infty(\mathcal{M}, \mathbf{R})$. As usual, we let vector fields be derivations of $C^\infty(\mathcal{M}, \mathbf{R})$ and we use the notation $F[\psi]$ to signify the result of applying this operator to a function $\psi \in C^\infty(\mathcal{M}, \mathbf{R})$. The product of two derivations F and G is defined as $(F \cdot G)[\psi] = F[G[\psi]]$, and we sometimes write this product just as juxtaposition. Note that even if both F and G are derivations, their composition is not. We define

$$\mathbf{F}(\bullet) = \mathbb{1}, \qquad \mathbf{F}(B_+(t_1, \ldots, t_\mu)) = \sum_{i_1,\ldots,i_\mu} \mathbf{F}(t_1)\big[f_{i_1}\big] \cdots \mathbf{F}(t_\mu)\big[f_{i_\mu}\big] E_{i_1} \cdots E_{i_\mu}.$$

As with vector fields, we can freeze the coefficients of these operators at any point $p \in \mathcal{M}$ and we define

$$\mathbf{F}_p(\bullet) = \mathbb{1}, \qquad \mathbf{F}_p(B_+(t_1, \ldots, t_\mu)) = \sum_{i_1,\ldots,i_\mu} \mathbf{F}(t_1)\big[f_{i_1}\big](p) \cdots \mathbf{F}(t_\mu)\big[f_{i_\mu}\big](p) E_{i_1} \cdots E_{i_\mu}.$$

This leads to a generalization of the B-series discussed in [8]. For any map $\mathbf{a} : T_O \to \mathbf{R}$ and $p \in \mathcal{M}$, we define the formal operator series

$$B(\mathbf{a}) = \sum_{t \in T_O} h^{|t|-1} \mathbf{a}(t) \mathbf{F}_p(t). \tag{7}$$

In what follows, we will frequently make calculation with series, these series should be always thought of as formal series without any concern about convergence.

The composition of frozen operators $\mathbf{F}_p(t)$ is multiplicative with respect to the product on trees defined above, that is, for any two trees u and v in T_O one has

$$\mathbf{F}_p(u)\mathbf{F}_p(v) = \mathbf{F}_p(u \cdot v). \tag{8}$$

2.2. Expansion of the exact solution

To expand the exact solution in a B-series, we need to consider the following series for the flow of a vector field:

$$\psi(\exp(tF)y) = \psi(y) + F[\psi](y) + \frac{1}{2!}(F \cdot F)[\psi](y) + \cdots = \operatorname{Exp}(tF)[\psi](y)$$

so we let $\operatorname{Exp}(tF)$ denote the exponential series of the operator tF. We have the following result from [20]:

Proposition 2.1. *The expansion of the exact flow $\psi(\exp(hF)y)$ can be expressed in a B-series $B(\mathbf{a})[\psi](y)$, where $\mathbf{a}(t) = \alpha(t)/(|t| - 1)!$, and where $\alpha(t)$ is defined recursively as follows:*

$$\alpha(\bullet) = 1 \qquad \textit{and} \qquad \alpha(t) = \alpha(B_+(t_1, \ldots, t_\mu)) = \prod_{\ell=1}^{\mu} \binom{\sum_{i=1}^{\ell} |t_i| - 1}{|t_\ell| - 1} \alpha(t_\ell). \tag{9}$$

2.3. Expansion of the numerical solution

Lemma 2.2. *Suppose that $\phi_{\mathbf{a}}$ and $\phi_{\mathbf{b}}$ are maps of $\mathcal{M}$ with B-series $B(\mathbf{a})$ and $B(\mathbf{b})$, where $\mathbf{a}(\bullet) = \mathbf{b}(\bullet) = 1$. Thus for any smooth function ψ we have*

$$\psi(\phi_{\mathbf{a}}(y)) = B(\mathbf{a})[\psi](y), \qquad \psi(\phi_{\mathbf{b}}(y)) = B(\mathbf{b})[\psi](y).$$

Then the composition of the maps $\phi_{\mathbf{a}} \circ \phi_{\mathbf{b}}$ has a B-series $B(\mathbf{ab})$ defined as

$$\mathbf{ab}(\bullet) = 1,$$

and for $t = B_+(t_1, \dots, t_\mu)$,

$$\mathbf{ab}(t) = \sum_{u \cdot v = t} \mathbf{a}(v)\mathbf{b}(u) = \sum_{k=0}^{\mu} \mathbf{a}(B_+(t_{k+1}, \dots, t_\mu))\mathbf{b}(B_+(t_1, \dots, t_k)).$$

Proof. We first set $z = \phi_{\mathbf{b}}(y)$, and calculate

$$\psi(\phi_{\mathbf{a}}(z)) = B(\mathbf{a})[\psi](z) = B(a)[\psi](\phi_{\mathbf{b}}(y)) = B(\mathbf{b})[B(\mathbf{a})[\psi]](y) := B(\mathbf{b})B(\mathbf{a})[\psi](\mathbf{y}).$$

Thus, $B(\mathbf{ab}) = B(\mathbf{b})B(\mathbf{a})$ and we multiply the two series and use (8) to obtain

$$\sum_{\substack{u \in T_O \\ v \in T_O}} h^{|u|-1}\mathbf{b}(u)h^{|v|-1}\mathbf{a}(v)\mathbf{F}_p(u)\mathbf{F}_p(v) = \sum_{\substack{u \in T_O \\ v \in T_O}} h^{|u \cdot v|-1}\mathbf{b}(u)\mathbf{a}(v)\mathbf{F}_p(u \cdot v)$$

A change of summation index yields the claimed result. □

Lemma 2.3. *Suppose that* $a = \phi_{\mathbf{a}}(p)$ *has a B-series* $B(\mathbf{a})$*. Then the frozen vector field* $F_a = \sum f_i(a)E_i \in \mathcal{V}$ *has the B-series* $F_a = B(\mathbf{F}_a)$ *where*

$$\mathbf{F}_a(\bullet) = 0$$
$$\mathbf{F}_a(B_+(t_1, \dots, t_\mu)) = 0, \qquad \mu \geqslant 2$$
$$\mathbf{F}_a(B_+(t)) = \mathbf{a}(t).$$

Proof

$$F_a = \sum_i f_i(\phi_{\mathbf{a}}(p))E_i = \sum_i \sum_{t \in T_O} h^{|t|-1}\mathbf{a}(t)\mathbf{F}_p(t)[f_i]E_i = \sum_{t \in T_O} h^{|t|-1}\mathbf{a}(t)\mathbf{F}_p(B_+(t)),$$

where we have used the recursive definition of the elementary differential operators. □

Lemma 2.4. *Let* $G \in \mathcal{V}$ *be any vector field with B-series of the form*

$$G = \sum_{t \in T_O} h^{|t|-1}\mathbf{G}(t)\mathbf{F}_p((t)).$$

Then, its h-flow $\exp(hG)p$ *has again a B-series* $B(\mathbf{g})$ *where*

$$\mathbf{g}(\bullet) = 1,$$
$$\mathbf{g}(B_+(t_1, \dots, t_\mu)) = \frac{1}{\mu!}\mathbf{G}(t_1)\cdots\mathbf{G}(t_\mu).$$

Proof. The exponential series gives, setting $u_i = B_+(t_i)$

$$\begin{aligned}\psi(\exp(hG)p) &= \sum_{\mu=0}^{\infty} \frac{h^\mu}{\mu!} G^\mu[\psi](p) \\ &= \sum_{\mu=0}^{\infty} \frac{h^\mu}{\mu!} \sum_{t_1,\dots t_\mu \in T_O} \prod_{i=1}^{\mu} h^{|t_i|-1}\mathbf{G}(t_i)\mathbf{F}_p(u_1)\cdots\mathbf{F}_p(u_\mu)[\psi](p).\end{aligned}$$

By (8) one has $\mathbf{F}_p(u_1)\cdots\mathbf{F}_p(u_\mu) = \mathbf{F}_p(B_+(t_1, \dots, t_\mu))$, and since the subtrees constitute an ordered set, every $t \in T_O$ appears precisely once in the form $t = B_+(t_1, \dots, t_\mu)$ as μ ranges from zero to infinity. Furthermore, since $h^\mu \prod_{i=1}^{\mu} h^{|t_i|-1} = h^{\sum_i t_i} = h^{|t|-1}$, we get by reorganizing the above expression

$$\psi(\exp(hG)p) = \sum_{t \in T_O} h^{|t|-1}\mathbf{g}(t)\mathbf{F}_p(t)[\psi](p)$$

with $\mathbf{g}(t)$ given as in the lemma. □

We now define

$$g_{r,0} = p \in \mathcal{M} \qquad \text{and} \qquad g_{r,j} = \exp\left(\sum_k \alpha_{r,j}^k F_k\right) g_{r,j-1}, \quad j = 1, \ldots, J,$$

so that $g_r = g_{r,J}$ in (5). Also, it is convenient to define $\alpha_{s+1,j}^k := \beta_j^k$ for $1 \leqslant k \leqslant s$ and $1 \leqslant j \leqslant J$. Then we can extend the above definition of $g_{r,j}$ also to $r = s+1$ such that $g_{s+1} := g_{s+1,J} = y_1$. From these definitions and the above lemmas, we have the result

Theorem 2.5. *Consider the commutator-free method (5) where we set $g_{s+1,J} := g_{s+1} = y_1$ and $g_{r,J} = g_r$, $1 \leqslant r \leqslant s$. Then $g_{r,j}$, $1 \leqslant r \leqslant s+1$, $1 \leqslant j \leqslant J$ have B-series $B(\mathbf{g}_{r,j})$ defined recursively as follows:*

$$\mathbf{g}_{r,j}(\bullet) = 1, \tag{10}$$

$$\mathbf{g}_{r,0}(t) = 0, \qquad \forall t : |t| > 1, \tag{11}$$

$$\mathbf{g}_{r,j}(B_+(t_1, \ldots, t_\mu)) = \sum_{k=0}^{\mu} \mathbf{g}_{r,j-1}(B_+(t_1, \ldots, t_k)) \cdot \mathbf{b}_{r,j}(B_+(t_{k+1}, \ldots, t_\mu)), \tag{12}$$

$$\mathbf{b}_{r,j}(\bullet) = 1, \qquad 1 \leqslant r \leqslant s+1, \quad 1 \leqslant j \leqslant J, \tag{13}$$

$$\mathbf{b}_{r,j}(B_+(t_1, \ldots, t_\mu)) = \frac{1}{\mu!} \mathbf{G}_{r,j}(t_1) \cdots \mathbf{G}_{r,j}(t_\mu), \tag{14}$$

$$\mathbf{G}_{r,j}(t) = \sum_{k=1}^{s} \alpha_{r,j}^k \mathbf{g}_{k,J}(t). \tag{15}$$

By combining proposition 2.1 and theorem 2.5, we obtain

Corollary 2.6. *A commutator-free Lie group method (5) has order of consistency q if and only if*

$$\mathbf{g}_{s+1,J}(t) = \frac{\alpha(t)}{(|t|-1)!}, \qquad \forall t : |t| \leqslant q+1.$$

Here $\mathbf{g}_{s+1,J}(t)$ is given recursively from theorem 2.5 and $\alpha(t)$ is given by (9).

Remark 2.7. It is possible to make the recursion formulae in the above theorem more in line with those that were derived for Crouch–Grossman schemes in [20]. By inserting (15) and (14) into (12), one gets

$$\mathbf{g}_{r,j}(B_+(t_1, \ldots, t_\mu)) = \sum_{k=0}^{\mu} \frac{1}{(\mu-k)!} \mathbf{g}_{r,j-1}(B_+(t_1, \ldots, t_k))$$
$$\times \sum_{\ell} \alpha_{r,j}^{\ell_{k+1}} \cdots \alpha_{r,j}^{\ell_\mu} \mathbf{g}_{\ell_{k+1},J}(t_{k+1}) \cdots \mathbf{g}_{\ell_\mu,J}(t_\mu), \tag{16}$$

where the last sum is over $\mu - k$ indices l_i all ranging from 1 to s. One may apply this formula repeatedly, starting with $j = J$ and the final result is

$$\mathbf{g}_{r,J}(B_+(t_1, \ldots, t_\mu)) = \sum_{\mathbf{j}<}^{J} \frac{1}{\mathbf{j}!} \sum_{\mathbf{k}}^{s} \alpha_{r,j_1}^{k_1} \cdots \alpha_{r,j_\mu}^{k_\mu} \mathbf{g}_{k_1,J}(t_1) \cdots \mathbf{g}_{k_\mu,J}(t_\mu), \qquad 1 \leqslant r \leqslant s+1,$$

where we have used the short-hand summation convention

$$\sum_{\mathbf{j}<}^{J} = \sum_{j_1=1}^{J} \sum_{j_2=j_1}^{J} \cdots \sum_{j_\mu=j_{\mu-1}}^{J} \qquad \text{and} \qquad \sum_{\mathbf{k}}^{s} = \sum_{k_1=1}^{s} \sum_{k_2=1}^{s} \cdots \sum_{k_\mu=1}^{s}.$$

The factorial of the multi-index $\mathbf{j}$ is defined as

$$\mathbf{j}! = q_1! \dots q_J!, \qquad q_i = (\#\text{occurrences of } i \text{ in } \mathbf{j}) \quad \sum q_i = \mu.$$

Example: $(1, 1, 2, 2, 3)! = 2! \cdot 2! \cdot 1! = 4$.

2.4. Simplifications for the case $J = 2$

We begin by presenting a very useful simplification of the formula for the quantities $\mathbf{g}_{r,j}$ as given in theorem 2.5, when $J = 2$.

Theorem 2.8. *Let $t_1, \dots, t_\mu$, $\mu \geqslant 2$ be any collection of trees in T_O. Define $t, u, v \in T_O$ such that $t = B_+(t_1, \dots, t_\mu)$, $u = B_+(t_1, \dots, t_{\mu-1})$ and $v = B_+(t_2, \dots, t_\mu)$. Then, if $J = 2$*

$$\mathbf{g}_r(t) = \mathbf{g}_{r,2}(t) = \frac{1}{\mu}\sum_{\ell=1}^{s}\big(\alpha_{r,1}^{\ell}\mathbf{g}_\ell(t_1)\mathbf{g}_r(v) + \alpha_{r,2}^{\ell}\mathbf{g}_\ell(t_\mu)\mathbf{g}_r(u)\big), \qquad 1 \leqslant r \leqslant s+1.$$

In particular one has for $r = s + 1$

$$\mathbf{y}_1(t) = \mathbf{g}_{s+1}(t) = \frac{1}{\mu}\sum_{\ell=1}^{s}\big(\beta_1^{\ell}\mathbf{g}_\ell(t_1)\mathbf{y}_1(v) + \beta_2^{\ell}\mathbf{g}_\ell(t_\mu)\mathbf{y}_1(u)\big).$$

Proof. By applying (16) twice, one gets

$$\mathbf{g}_r(t) = \frac{1}{\mu!}\sum_{k=0}^{\mu}\binom{\mu}{k}\sum_{\ell}\alpha_{r,1}^{\ell_1}\cdots\alpha_{r,1}^{\ell_k}\alpha_{r,2}^{\ell_{k+1}}\cdots\alpha_{r,2}^{\ell_\mu}\mathbf{g}_{\ell_1}(t_1)\cdots\mathbf{g}_{\ell_\mu}(t_\mu).$$

One may now split this sum into two parts, and use the identity

$$\binom{\mu}{k} = \binom{\mu-1}{k-1} + \binom{\mu-1}{k}, \qquad 1 \leqslant k \leqslant \mu - 1.$$

We get

$$\begin{aligned}
\mathbf{g}_r(t) = \frac{1}{\mu!}\Bigg(&\sum_{k=1}^{\mu}\sum_{\ell}\alpha_{r,1}^{\ell_1}\mathbf{g}_{\ell_1}(t_1)\binom{\mu-1}{k-1}\alpha_{r,1}^{\ell_2}\cdots\alpha_{r,1}^{\ell_k}\alpha_{r,2}^{\ell_{k+1}}\cdots\alpha_{r,2}^{\ell_\mu}\mathbf{g}_{\ell_2}(t_2)\cdots\mathbf{g}_{\ell_\mu}(t_\mu) \\
&+\sum_{k=0}^{\mu-1}\sum_{\ell}\alpha_{r,2}^{\ell_\mu}\mathbf{g}_{\ell_\mu}(t_\mu)\binom{\mu-1}{k}\alpha_{r,1}^{\ell_1}\cdots\alpha_{r,1}^{\ell_k}\alpha_{r,2}^{\ell_{k+1}}\cdots\alpha_{r,2}^{\ell_\mu}\mathbf{g}_{\ell_1}(t_1)\cdots\mathbf{g}_{\ell_{\mu-1}}(t_{\mu-1})\Bigg), \\
= \frac{1}{\mu}\Bigg(&\sum_{\ell_1=1}^{s}\alpha_{r,1}^{\ell_1}\mathbf{g}_{\ell_1}(t_1)\mathbf{g}_r(v) + \sum_{\ell_\mu=1}^{s}\alpha_{r,2}^{\ell_\mu}\mathbf{g}_{\ell_\mu}(t_\mu)\mathbf{g}_r(u)\Bigg).
\end{aligned}$$

□

3. Minimal sets of order conditions

We have seen that B-series of the form (7) are used to formally express objects of very different kinds, such as maps and vector fields. This suggests that in the set of maps from T_O to $\mathbf{R}$, there are subsets representing each object type. In order to characterize these subsets, we begin by interpreting the trees and expansions in a strictly algebraic fashion.

Let $A_- \subset T_O$ be the set of trees of the form $B_+(t)$ for $t \in T_O$, and let $A = A_- \cup \{\bullet\}$. Any tree $t = B_+(t_1, \dots, t_\mu) \in T_O$ can now be considered as a word of the *alphabet* A, in the sense that the finite sequence $B_+(t_1), \dots, B_+(t_\mu)$ of elements of A, forms the word $B_+(t_1, \dots, t_\mu)$. With the concatenation product defined on trees in section 2.1, we obtain the whole set T_O as the free monoid on A, see for instance [21]. The tree $\bullet$ serves as the identity element. We may now extend this structure to an $\mathbf{R}$-algebra $\mathbf{R}T_O$ which we for notational convenience denote $\mathcal{B}$. Its elements are the formal series on A, and it is in fact known to be the *free associative* $\mathbf{R}$*-algebra* on the set A. Denoting by $(P, t) \in \mathbf{R}$ the coefficient of the tree t in the series P, we define the product of two series S and T to be the series with coefficients

$$(ST, t) = \sum_{t=uv} (S, u)(T, v).$$

Next, we note that all integration methods considered here are derived by composing exponentials of linear combinations of frozen vector fields. According to lemma 2.3, these linear combinations have expansions with coefficients which are zero on trees not belonging to A_-. Compositions of exponentials of such series can be expressed formally as the exponential of one single vector field through the Baker–Campbell–Hausdorff formula; thus we conclude that every map considered here is the exponential of a vector field whose expansion is in the free Lie algebra $\mathfrak{g}$ on the set $A_- \subset T_O$.

We define the following three subsets of $\mathcal{B}$:

- The subspace $\mathfrak{g} \subset \mathcal{B}$ which is the free Lie algebra on the set A.
- $\mathcal{V} \subset \mathfrak{g}$ is the subspace of $\mathfrak{g}$ consisting of series S such that

$$(S, t) = 0 \qquad \text{whenever } t \notin A_-.$$

- G is the *Malcev* group of exponential series $T = \exp(S)$, $S \in \mathfrak{g}$. In particular, if $T \in G$ then $(T, \bullet) = 1$.

The characterization of this Lie algebra is well known, see for instance [21]. We define the coproduct $\Delta : \mathcal{B} \to \mathcal{B} \otimes \mathcal{B}$ to be the unique homomorphism of $\mathbf{R}$-algebras sending $\bullet$ to $(\bullet \otimes \bullet)$ and such that

$$\Delta(t) = \bullet \otimes t + t \otimes \bullet \qquad \text{for any } t \in A_-.$$

Writing this out for an arbitrary tree $t = B_+(t_1, \ldots, t_\mu)$, one gets

$$\Delta(t) = \sum_{f \subseteq B_-(t)} B_+(f) \otimes B_+(f^c),$$

where the sum is over all subforests of $B_-(t)$ including the empty set and $B_-(t)$ itself and where f^c is the complement of f in $B_-(t)$. The ordering of the subforests f and f^c is inherited from the ordered set $B_-(t)$.

The Lie algebra $\mathfrak{g}$ is now characterized as

$$\mathfrak{g} = \{S \in \mathcal{B} : \Delta(S) = \bullet \otimes S + S \otimes \bullet\}.$$

By dualizing this relation, one obtains internal relations between the coefficients (S, t) of a series $S \in \mathfrak{g}$. One gets for any $t_1 \otimes t_2 \in \mathcal{B} \otimes \mathcal{B}$

$$(S, t_1 ⧢ t_2) t_1 \otimes t_2 = 0,$$

see [21] for a proper definition of the shuffle product ⧢. So we may conclude that the dependences among the coefficients of a Lie series $S \in \mathfrak{g}$ occur for trees which are identical modulo a permutation of subtrees. Using, yet again, classical theory of free Lie algebras, one may characterize this dependency by a generalized Witt formula counting, for a given tree t, the dimension of the subspace of $\mathfrak{g}$ spanned by the set of trees obtained from permuting the subtrees of t. Consider the equivalence class $[t]$ characterized by a set of ν distinct subtrees

$t_i \in T_O$, $i = 1, \dots, \nu$, where there are exactly α_i occurrences of the subtree t_i. From Bourbaki [1], we find that the subspace spanned by the set of trees in $[t]$ has dimension

$$c(\alpha) = 1/|\alpha| \sum_{d|\alpha} \mu(d) \frac{(|\alpha|/d)!}{(\alpha/d)!}. \tag{17}$$

This relation will be useful in the following in selecting a minimal set of order conditions. Some examples are

$$\begin{aligned} &c(n) = 0, && n > 1 \\ &c(n, 1) = 1, && n > 0, \\ &c(n, 1, 1) = n + 1, && n > 0, \\ &c(n, 2) = \left\lfloor \frac{n+1}{2} \right\rfloor, && n > 0. \end{aligned} \tag{18}$$

We have seen that there is a natural grading on $\mathcal{B}$ corresponding to the number of nodes in each tree, defining the grade $\nu(t) = |t| - 1$ one sees that $\nu(u \cdot v) = |u \cdot v| - 1 = |u| + |v| - 2 = \nu(u) + \nu(v)$. One may decompose the spaces $\mathcal{B}$ and $\mathfrak{g}$ according to this grading as

$$\mathcal{B} = \coprod_{n\geqslant 0} \mathcal{B}_n, \qquad \mathfrak{g} = \coprod_{n\geqslant 1} \mathfrak{g}_n, \qquad \mathfrak{g}_n = \mathfrak{g} \cap \mathcal{B}_n.$$

Clearly $\dim \mathcal{B}_n$ is the number of ordered rooted trees with exactly $n+1$ nodes; it is well known (see, e.g. [5]) that this number is given as the Catalan number

$$\dim \mathcal{B}_n = C_n = \frac{1}{n+1}\binom{2n}{n}, \tag{19}$$

having generating function

$$g(T) = \sum_{n=0}^{\infty} C_n T^n = \frac{2}{1 + \sqrt{1 - 4T}}. \tag{20}$$

We prove the following result:

Theorem 3.1

$$\dim \mathfrak{g}_n = \nu_n = \frac{1}{2n} \sum_{d|n} \mu(d) \binom{2n/d}{n/d},$$

where $\mu(d)$ is the Möbius function defined for any positive integer as $\mu(1) = 1$, $\mu(d) = (-1)^p$ when d is the product of p distinct primes, and $\mu(d) = 0$ otherwise. The sum is over all positive integers which divide n, including 1 and n.

Proof. This formula is well known in several different contexts, for instance, it counts the number of balanced Lyndon words [1] and has been used recently in the context of geometric integration in [10] and [19]. The proof is mainly based on the Poincaré–Birkhoff–Witt (PBW) theorem concerning the *enveloping algebra* of the free Lie algebra $\mathfrak{g}$. It is well known [22, theorem 3.2.8, p. 174] that $\mathcal{B}$ is also the enveloping algebra of $\mathfrak{g}$. A standard way of finding the dimensions ν_n is to consider the dimensions $\dim \mathcal{B}_n$. Viewing $\mathcal{B}$ as the enveloping algebra of $\mathfrak{g}$, one has from the PBW theorem

$$\sum_{m=0}^{\infty} \dim \mathcal{B}_m T^m = \prod_{n=1}^{\infty} \left(\sum_{r=0}^{\infty} T^{nr} \right)^{\nu_n} = \prod_{n=1}^{\infty} (1 - T^n)^{-\nu_n} \tag{21}$$

which we now just need to compare to (20) and solve for ν_n.

We take logarithms of both expressions and use the expansion $-\log(1-x) = \sum_{k=1}^{\infty} x^k/k$

$$\sum_{n=1}^{\infty} \nu_n \sum_{k=1}^{\infty} \frac{1}{k} T^{nk} = \log g(T) = \sum_{m=1}^{\infty} \frac{1}{2m}\binom{2m}{m} T^m,$$

where the Taylor coefficients of $\log g(T)$ are found, for instance, by using the relation $(\log g(T))' = g'(T)/g(T) = \frac{1}{2}(g'(T) - (g(T)-1)/T)$ which is easily verified. Comparing equal powers we get

$$\sum_{d|m} \nu_d \frac{d}{m} = \frac{1}{2m}\binom{2m}{m}.$$

The Möbius inversion formula thus yields

$$n\nu_n = \sum_{d|n} \mu(d) \frac{1}{2}\binom{2n/d}{n/d}.$$

□

The maps we consider here have B-series in $\mathcal{B}$ interpreted as exponentials of series in $\mathfrak{g}$. It is easy to prove that if $T = \exp(S)$ with $S \in \mathfrak{g}$, then T satisfies the following relation in terms of the above coproduct:

$$\Delta(T) = T \otimes T.$$

This relation can also be characterized in terms of the *shuffle* product on $\mathcal{B}$ by

$$(T, u ⧢ v) = (T, u)(T, v).$$

4. Examples and implementation issues

4.1. Order conditions up to order 4

The eight classical order conditions up to order 4 are well known, and given as

Order	Condition	Order	Condition
1	$\sum_r b^r = 1,$	4	$\sum_r b^r c_r^3 = \frac{1}{4},$
2	$\sum_r b^r c_r = \frac{1}{2},$	4	$\sum_{r,k} b^r c_r a_k^r c_k = \frac{1}{8},$
3	$\sum_r b^r c_r^2 = \frac{1}{3},$	4	$\sum_{r,k} b^r a_k^r c_k^2 = \frac{1}{12},$
3	$\sum_{r,k} b^r a_r^k c_k = \frac{1}{6},$	4	$\sum_{r,k,m} b^r a_r^k a_k^m c_m = \frac{1}{24}.$

(22)

These must be fulfilled also by the commutator-free schemes (5) with

$$b^r = \sum_j \beta_j^r, \qquad a_r^k = \sum_j \alpha_{r,j}^k. \tag{23}$$

To simplify the notation in what follows, we shall work with covectors in $(\mathbf{R}^s)^*$ whose components are the upper indices, as

$$\beta_j = \left[\beta_j^1, \ldots, \beta_j^s\right]$$

and we use tensor product notation to indicate multilinear mappings on $\mathbf{R}^s \times \cdots \times \mathbf{R}^s$ as for instance

$$(\beta_j \otimes \beta_m)(u, v) = \sum_{k_1,k_2} \beta_j^{k_1} \beta_j^{k_2} u_{k_1} v_{k_2}.$$

We next introduce the $(\mu, 0)$-tensor

$$\mathbf{t}_\mu = \sum_{\mathbf{j}<} \frac{1}{\mathbf{j}!} \beta_{j_1} \otimes \cdots \otimes \beta_{j_\mu}, \qquad \mu \geqslant 1. \tag{24}$$

We have for example

$$\mathbf{t}_2 = \sum_{j_1=1}^{J} \left(\beta_{j_1} \otimes \left(\frac{1}{2} \beta_{j_1} + \sum_{j_2 > j_1} \beta_{j_2} \right) \right). \tag{25}$$

There are no additional order conditions for orders 1 and 2. For order 3, however, one must take into account the order condition associated with either of the two trees

 or .

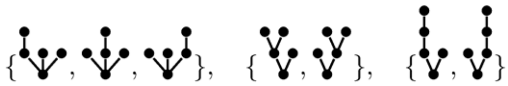
Denote by $\mathbf{1} = [1, \ldots, 1]^T$ the s-vector of ones and $\mathbf{c}^q = \left[c_1^q, \ldots, c_s^q\right]^T$ the qth power of the abscissae in the scheme, and $\mathbf{c} = \mathbf{c}^1$. The third-order non-classical condition is

$$\mathbf{t}_2(\mathbf{1}, \mathbf{c}) = 2\mathbf{t}_2(\mathbf{c}, \mathbf{1}) = \tfrac{1}{3}. \tag{26a}$$

In the case that there are two exponentials in the final stage, one can use theorem 2.8 and replace (26a) by the condition

$$\beta_1(\mathbf{c}) + \tfrac{1}{2}\beta_2(\mathbf{1}) = \tfrac{1}{3}. \tag{26b}$$

As for the fourth-order condition, one first sees that there are 14 trees with five nodes. The two trees  and  can be discarded, and among the subsets



one needs to include exactly one tree. The corresponding general condition and the version valid in the case of two exponential are, respectively

$$\mathbf{t}_3(\mathbf{c}, \mathbf{1}, \mathbf{1}) = \tfrac{1}{24} \text{ (general)}, \tag{27a}$$

$$\tfrac{1}{6}\beta_1(\mathbf{c}) + \tfrac{1}{18}\beta_2(\mathbf{1}) = \tfrac{1}{24} \text{ (two exponentials)}. \tag{27b}$$

Choosing the first tree of the second set, we get the conditions

$$\mathbf{t}_2\left(\tfrac{1}{2}\mathbf{c}^2, \mathbf{1}\right) = \tfrac{1}{24} \text{ (general)}, \tag{28a}$$

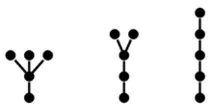
$$\tfrac{1}{4}\beta_1(\mathbf{c}^2) + \tfrac{1}{12}\beta_2(\mathbf{1}) = \tfrac{1}{24} \text{ (two exponentials)}, \tag{28b}$$

and from the first condition of the last set, we get

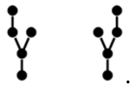
$$\mathbf{t}_2(\mathbf{ac}, \mathbf{1}) = \tfrac{1}{24} \text{ (general)}, \tag{29a}$$

$$\tfrac{1}{2}\beta_1(\mathbf{ac}) + \tfrac{1}{12}\beta_2(\mathbf{1}) = \tfrac{1}{24} \text{ (two exponentials)}. \tag{29b}$$

The remaining five trees are related to the classical order conditions (22). The first, third and fourth conditions of order 4 correspond, respectively, to the trees

,

whereas the second fourth-order condition of (22) is the sum of the conditions corresponding to each of the two trees



(30)

So, given that the classical order conditions have been imposed, it suffices to consider one of the two above trees and the order condition is

$$\sum_r b^r \mathbf{T}_{2,r}(\mathbf{c}, 1) = \frac{1}{24} \text{ (general)} \tag{31a}$$

where the $(\mu, 0)$-tensor $\mathbf{T}_{\mu,r}$ is formed as

$$\mathbf{T}_{\mu,r} = \sum_{\mathbf{j}<} \frac{1}{\mathbf{j}!} \alpha_{j_1,r} \otimes \cdots \otimes \alpha_{j_\mu,r}. \tag{32}$$

The condition (31a) is actually the first one to involve the non-classical coupling coefficients $\alpha^k_{r,j}$ of the scheme, thus this condition is responsible for the necessity of having more than one exponential in at least one of the internal stages. Setting $J = 1$ in all internal stages would yield conflicting conditions corresponding to the two trees (30). If we allow instead at most two exponentials in the internal stages, we get the condition

$$\frac{1}{2}\left(\sum_{r,\ell} b^r c_r \alpha^\ell_{r,1} c_\ell + \sum_{r,\ell,m} b^r a^\ell_r c_\ell \alpha^m_{\ell,2}\right) = \frac{1}{24} \text{ (two exponentials).} \tag{31b}$$

A useful strategy for constructing commutator-free schemes is to start with an underlying classical Runge–Kutta scheme which satisfies the classical order conditions (22) up to order $p \leqslant 4$. Then, there is one extra condition for schemes order 3, and four additional ones for order 4. The equations marked 'a' may be used for the general case, and those marked 'b' may be used when there are at most two exponentials. For schemes of order 3, three stages are needed and the update stage must contain (at least) two exponentials in order to satisfy (26b). On the other hand, this extra exponential provides three parameters. For schemes of order 4 satisfying the classical conditions, the β-parameters are, in the case of two exponentials in the update stage, involved in (26b), (27b), (28b) and (29b). We observe that these four equations immediately yield

$$\beta_1(\mathbf{1}) = \tfrac{1}{2}, \qquad \beta_1(\mathbf{c}) = \tfrac{1}{12}, \qquad \beta_1(\mathbf{c}^2) = 0, \qquad \beta_1(\mathbf{ac}) = 0. \tag{33}$$

The condition (31b) calls for two exponentials in one of the internal stages. Adding another one in stage r gives $r - 1$ extra parameters.

4.2. Reusing exponentials

Suppose the commutator-free scheme (5) is explicit. In [3] it was suggested that whenever more than one exponential is to be included in a stage, it may be possible to reuse exponential calculations performed in previous stages. If the coefficients can be chosen such that for some $1 \leqslant r < \hat{r} \leqslant s + 1$ and $j^* \geqslant 1$,

$$\alpha^k_{r,j} = \alpha^k_{\hat{r},j}, \qquad 1 \leqslant k \leqslant s, \quad 1 \leqslant j \leqslant j^*,$$

then

$$p^* = \exp\left(\sum_k \alpha^k_{r,j^*} F_k\right) \cdots \exp\left(\sum_k \alpha^k_{r,1} F_k\right)(p)$$

can be stored, and subsequently g_r, $g_{\hat{r}}$ can be computed from

$$g_r = \exp\left(\sum_k \alpha^k_{r,J} F_k\right) \cdots \exp\left(\sum_k \alpha^k_{r,j^*+1} F_k\right)(p^*),$$

$$g_{\hat{r}} = \exp\left(\sum_k \alpha^k_{\hat{r},J} F_k\right) \cdots \exp\left(\sum_k \alpha^k_{\hat{r},j^*+1} F_k\right)(p^*).$$

Thereby the cost of j^* calculations of the exponential map is saved. In the case that one may allow for storing separate exponential maps (as, e.g. matrices), there are further possibilities for reuse.

The schemes of order 3 are discussed in detail in [3].

4.2.1. Explicit fourth-order schemes with four stages. We refer to [8, p. 138] for a complete classification of fourth-order classical Runge–Kutta schemes. There exists one two-parameter family and three one-parameter families of such schemes. We shall allow exactly two exponentials in the update stage, and assume that there is an underlying classical Runge–Kutta scheme with coefficients b^r, a^k_r as in (23) satisfying the classical order conditions (22). The conditions (33) uniquely determine all the β^k_1. It is impossible to reuse an exponential in the update stage because the explicitness of the scheme would require $\beta^4_1 = 0$, leading to an inconsistency. As mentioned above, one extra exponential is needed in one of the internal stages. We include this in the last stage to maximize the number of free parameters and allow for reusing an exponential from one of the first two stages. We have at our disposal the coefficients $\alpha^1_{4,1}, \ldots, \alpha^3_{4,1}$, the $\alpha^k_{4,2}$ being determined by (23). It is natural to try to make the exponential from the second or third stage coincide with the rightmost exponential in the fourth stage, setting

$$\alpha^k_{4,1} = a^k_r, \qquad r = 2 \text{ or } 3, \qquad k = 1, \ldots, r-1. \tag{34}$$

This requirement is rather restrictive; it completely determines all the $\alpha^k_{4,j}$ coefficients when the underlying classical scheme is given.

However, equation (31*b*) must still hold and this leads to further conditions on the classical underlying coefficients

$$b^4(a_{42}c_2 + a_{43}c_3)c_2 = \tfrac{1}{24}, \qquad \text{if } r = 2 \text{ in (34)}$$

or

$$b^4(a_{42}c_2 + a_{43}c_3)c_3 - b^4 a_{32}c_2 = \tfrac{1}{24}, \qquad \text{if } r = 3 \text{ in (34)}.$$

In reusing the exponential from the second stage, one can choose $c_2 \notin \{0, 1/3, 1/4, 1\}$ and then set

$$c_3 = \frac{3c_2 - 1}{4c_2 - 1}.$$

The classical RK4 scheme of Kutta with $c_2 = c_3 = \frac{1}{2}$ was given as an example of such schemes in [3]; it is the leftmost scheme of figure 1. It is interesting to observe also that with the choice of linear space $\mathcal{V}$ as in (3) the internal stages of this scheme coincide with an exponential integrator presented by Cox and Matthews [6]. Note that the famous 3/8-rule of Kutta having $c_2 = 1/3$, $c_3 = 2/3$ cannot be used in this way. Reusing the exponential of the third stage is also possible. Incidentally, it happens that the RK4 scheme also allows for a reuse of the exponential in the third stage, see the rightmost scheme of figure 1.

There exists one other confluent scheme which reuses this exponential namely the one given in figure 2.

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & \frac{1}{2} & 0 & 0 & \\
 & -\frac{1}{2} & 0 & 1 & \\
\hline
 & \frac{1}{4} & \frac{1}{6} & \frac{1}{6} & -\frac{1}{12} \\
 & -\frac{1}{12} & \frac{1}{6} & \frac{1}{6} & \frac{1}{4}
\end{array}
\qquad
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & 0 & \frac{1}{2} & 0 & \\
 & 0 & -\frac{1}{2} & 1 & \\
\hline
 & \frac{1}{4} & \frac{1}{6} & \frac{1}{6} & -\frac{1}{12} \\
 & -\frac{1}{12} & \frac{1}{6} & \frac{1}{6} & \frac{1}{4}
\end{array}
\tag{35}
$$

Figure 1. Commutator-free schemes of order 4 based on the classical RK4 scheme, reusing exponentials from second and third stages, respectively.

$$
\begin{array}{c|cccc}
0 & & & & \\
1 & 1 & & & \\
\frac{1}{2} & \frac{3}{8} & \frac{1}{8} & & \\
1 & \frac{3}{8} & \frac{1}{8} & 0 & \\
 & -\frac{1}{8} & -\frac{3}{8} & 1 & \\
\hline
 & \frac{1}{4} & \frac{1}{12} & \frac{1}{3} & -\frac{1}{6} \\
 & -\frac{1}{12} & -\frac{1}{4} & \frac{1}{3} & \frac{1}{2}
\end{array}
$$

Figure 2. Commutator-free schemes of order 4 based on a confluent scheme, reusing exponentials from the third stage.

All other schemes which reuse the exponential from the third stage must have c_2 and c_3 which satisfy the relation

$$2(3c_2 - 2)c_3^2 + \left(3 + 2c_2^2 - 6c_2\right)c_3 + 3c_2 - 2c_2^2 = 1.$$

Unfortunately, the procedure presented here cannot be applied to obtain commutator-free generalizations of classical schemes of order 5 and higher because the composition of more than two exponentials is required. There are, for instance, a total of 25 conditions of order 5 according to theorem 3.1. Of these, 11 involve the β-coefficients of the update stage. Fifth-order classical explicit Runge–Kutta schemes have at least six stages, thus three exponentials ($J = 3$) in the update stage would add 12 parameters. The conditions can however not be made linear when $J = 3$.

We have presented a general order theory for the commutator-free schemes introduced in [3]. Several new schemes of order 4 are easily obtained from this discussion. Much work still remains for constructing schemes of higher order, but the theory presented here can be used to write down the order conditions to any order.

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