Found Comput Math (2010) 10: 407–427
DOI 10.1007/s10208-010-9065-1

FOUNDATIONS OF COMPUTATIONAL MATHEMATICS
The Journal of the Society for the Foundations of Computational Mathematics

Algebraic Structures of B-series

Philippe Chartier · Ernst Hairer · Gilles Vilmart

Received: 10 February 2009 / Revised: 10 November 2009 / Accepted: 16 February 2010 /
Published online: 24 March 2010

Abstract B-series are a fundamental tool in practical and theoretical aspects of numerical integrators for ordinary differential equations. A composition law for B-series permits an elegant derivation of order conditions, and a substitution law gives much insight into modified differential equations of backward error analysis. These two laws give rise to algebraic structures (groups and Hopf algebras of trees) that have recently received much attention also in the non-numerical literature. This article emphasizes these algebraic structures and presents interesting relationships among them.

Keywords B-series · Rooted trees · Composition law · Substitution law · Butcher group · Hopf algebra of trees · Coproduct · Antipode · P-series · S-series

Mathematics Subject Classification (2000) 65L06 · 65P10 · 37C10 · 16W30

Communicated by Arieh Iserles.

P. Chartier
INRIA Rennes, ENS Cachan Bretagne, Campus Ker-Lann, av. Robert Schumann, 35170 Bruz, France
e-mail: Philippe.Chartier@inria.fr

E. Hairer
Section de Mathématiques, Université de Genève, 2-4 rue du Lièvre, 1211 Genève 4, Switzerland
e-mail: Ernst.Hairer@unige.ch

G. Vilmart (✉)
Section de Mathématiques, École Polytechnique Fédérale de Lausanne, SB MATHICSE ANMC, Station 8, 1015 Lausanne, Switzerland
e-mail: Gilles.Vilmart@epfl.ch

1 Introduction

Let us consider systems of differential equations

$$\dot{y} = f(y) \tag{1}$$

with smooth vector field $f(y)$. Since the work of Cayley [10] and Merson [36] it is known that the expressions arising in the derivatives of its solution, $\ddot{y} = (f'f)(y)$, $\dddot{y} = (f''(f,f))(y) + (f'f'f)(y)$, are in one-to-one correspondence with rooted trees. It is therefore natural to consider formal series of the form

$$\begin{aligned} B(a,hf,y) = a(\emptyset)y + ha(\bullet)f(y) + h^2a([\bullet])(f'f)(y) + \frac{h^3}{2}a([\bullet,\bullet])\big(f''(f,f)\big)(y) \\ + h^3a\big([[\bullet]]\big)(f'f'f)(y) + h^4a\big([\bullet,[\bullet]]\big)\big(f''(f,f'f)\big)(y) + \cdots \end{aligned} \tag{2}$$

with scalar coefficients $a(\emptyset)$, $a(\bullet)$, $a([\bullet])$, etc. The exact solution of (1) is of this form with $a(\emptyset) = a(\bullet) = 1$, $a([\bullet]) = 1/2$, $a([\bullet,\bullet]) = 1/3$, etc. In his fundamental work on order conditions, Butcher discovered in the 1960s (culminating in the seminal article [5]) that the numerical solution of a Runge–Kutta method is also a series of the form (2) with $a(\tau)$ depending only on the coefficients of the method. Hairer and Wanner [29] considered series (2) with arbitrary coefficients and called them B-series.[1] They applied them to the elaboration of order conditions for general multi-value methods. B-series and extensions thereof are now exposed in various textbooks and articles, possibly with different normalizations; see e.g., [6, 26].

B-series play an important role in the study and construction of numerical integrators. This is a consequence of the following two operations on B-series:

- Composition law [5, 29]. For $b(\emptyset) = 1$, a B-series considered as a mapping $y \mapsto B(b,hf,y)$ is $\mathcal{O}(h)$-close to the identity. It is therefore possible to replace y in (2) with $B(b,hf,y)$, and to expand all expressions around y. Interestingly, the result is again a B-series and we have

$$B\big(a,hf,B(b,hf,y)\big) = B(b\cdot a,hf,y). \tag{3}$$

- Substitution law [14, 15]. For $b(\emptyset) = 0$, the B-series $B(b,hf,y)$ is a vector field that is a perturbation of $hf(y)$, multiplied by the scalar $b(\bullet)$. Therefore, we can substitute the vector field $B(b,hf,\cdot)$ for hf in (2). Also in this case we obtain a B-series, which we denote

$$B\big(a,B(b,hf,\cdot),y\big) = B(b\star a,hf,y). \tag{4}$$

[1] Originally called a Butcher series.

A straightforward computation yields for the composition law $(b\cdot a)(\emptyset)=a(\emptyset)$ and

$$
\begin{aligned}
(b\cdot a)(\bullet) &= a(\emptyset)b(\bullet)+a(\bullet),\\
(b\cdot a)([\bullet]) &= a(\emptyset)b([\bullet])+a(\bullet)b(\bullet)+a([\bullet]),\\
(b\cdot a)([\bullet,\bullet]) &= a(\emptyset)b([\bullet,\bullet])+a(\bullet)b(\bullet)^2+2a([\bullet])b(\bullet)+a([\bullet,\bullet]),\\
(b\cdot a)([[\bullet]]) &= a(\emptyset)b([[\bullet]])+a(\bullet)b([\bullet])+a([\bullet])b(\bullet)+a([[\bullet]]).
\end{aligned}
\tag{5}
$$

Similarly, for the substitution law we obtain $(b\star a)(\emptyset)=a(\emptyset)$ and

$$
\begin{aligned}
(b\star a)(\bullet) &= a(\bullet)b(\bullet),\\
(b\star a)([\bullet]) &= a(\bullet)b([\bullet])+a([\bullet])b(\bullet)^2,\\
(b\star a)([\bullet,\bullet]) &= a(\bullet)b([\bullet,\bullet])+2a([\bullet])b(\bullet)b([\bullet])+a([\bullet,\bullet])b(\bullet)^3,\\
(b\star a)([[\bullet]]) &= a(\bullet)b([[\bullet]])+2a([\bullet])b(\bullet)b([\bullet])+a([[\bullet]])b(\bullet)^3.
\end{aligned}
\tag{6}
$$

General formulae for both laws will be given in Sect. 3 below.

The composition law is an important tool for the construction of various integration methods, such as Runge–Kutta methods, general linear methods, Rosenbrock methods, multi-derivative methods, etc. It allows the derivation of the order conditions for arbitrarily high orders in an elegant way avoiding tedious series expansions [27, 30]. Another application is the composition of different numerical integrators yielding higher accuracy: effective order or pre- and post-processing of composition methods [1, 4].

Applications of the substitution law are more recent and mainly in connection with structure-preserving algorithms (geometric numerical integration). This law gives much insight into the modified differential equation of backward error analysis [26], and it is the main ingredient for the construction of modifying integrators [15].

1.1 Group and Monoid Structures

Let $T=\{\bullet,[\bullet],[\bullet,\bullet],\ldots\}$ be the set of rooted trees, and consider the set $T_0=T\cup\{\emptyset\}$ including the empty tree. The set of mappings

$$G_C=\big\{a\colon T_0\to\mathbb{R};\, a(\emptyset)=1\big\} \tag{7}$$

with the product (5) of the composition law is a group. The identity is the element that corresponds to the B-series $B(a,hf,y)=y$. Associativity follows from that of the composition of mappings and the existence of an inverse is obtained from the explicit formulae for the product. The group G_C has been introduced in [5] and is called the Butcher group in [29].

In a similar way, the substitution law (6) makes the set

$$G_S=\big\{a\colon T_0\to\mathbb{R};\, a(\emptyset)=0\big\} \tag{8}$$

a monoid. It is a monoid of vector fields and has first been considered in [14]. The identity element is the mapping that corresponds to the B-series $B(a,hf,y)=hf(y)$.

Invertible elements in G_S are those with $a(\bullet) \neq 0$ and yield the group

$$G_S^* = \{a\colon T_0 \to \mathbb{R};\, a(\emptyset) = 0,\, a(\bullet) \neq 0\}. \tag{9}$$

1.2 Hopf Algebras of Trees

Independently of the theory of B-series, Connes and Moscovici [20] in the context of non-commutative geometry, and Connes and Kreimer [18, 19] in the theory of renormalization consider a Hopf algebra of rooted trees whose co-product is for the first trees given by $\Delta_{\mathrm{CK}}(\emptyset) = \emptyset \otimes \emptyset$ and

$$\begin{aligned}
\Delta_{\mathrm{CK}}(\bullet) &= \bullet \otimes \emptyset + \emptyset \otimes \bullet, \\
\Delta_{\mathrm{CK}}([\bullet]) &= [\bullet] \otimes \emptyset + \bullet \otimes \bullet + \emptyset \otimes [\bullet], \\
\Delta_{\mathrm{CK}}([\bullet\bullet]) &= [\bullet\bullet] \otimes \emptyset + \bullet\bullet \otimes \bullet + 2\,\bullet \otimes [\bullet] + \emptyset \otimes [\bullet\bullet], \\
\Delta_{\mathrm{CK}}([[\bullet]]) &= [[\bullet]] \otimes \emptyset + [\bullet] \otimes \bullet + \bullet \otimes [\bullet] + \emptyset \otimes [[\bullet]].
\end{aligned} \tag{10}$$

Brouder [2, 3] (and also implicitly Dür [21]) noticed the close connection between this co-product and the product (5) of the composition law.

Indeed, it is obtained from (5) by writing the argument of the mapping a to the right of the $\otimes$ sign, and those of the mapping b to the left of it. To the last terms in (5), which do not contain any $b(\tau)$, one adds the trivial factor $b(\emptyset) = 1$.

It is not surprising that a similar connection holds also for the substitution law. Inspired by the work [14], Calaque et al. [8] introduced a co-product which, for the first trees, is given by

$$\begin{aligned}
\Delta_{\mathrm{CEM}}(\bullet) &= \bullet \otimes \bullet, \\
\Delta_{\mathrm{CEM}}([\bullet]) &= [\bullet] \otimes \bullet + \bullet^2 \otimes [\bullet], \\
\Delta_{\mathrm{CEM}}([\bullet\bullet]) &= [\bullet\bullet] \otimes \bullet + 2\bullet [\bullet] \otimes [\bullet] + \bullet^3 \otimes [\bullet\bullet], \\
\Delta_{\mathrm{CEM}}([[\bullet]]) &= [[\bullet]] \otimes \bullet + 2\bullet [\bullet] \otimes [\bullet] + \bullet^3 \otimes [[\bullet]].
\end{aligned} \tag{11}$$

It gives rise to a new Hopf algebra of trees.

1.3 Outline of the Article

The aim of this paper, which can be seen as a mixture of survey and research article, is to discuss the composition and substitution laws, to explain their fundamental role in numerical analysis, and to explore their common algebraic structure and relationships.

Section 2 rigorously introduces trees and B-series, and in particular also ordered subtrees and partitions of trees. The composition and substitution laws are discussed in Sect. 3, including explicit formulae for arbitrary trees and applications in numerical analysis. Various relations between the two laws are explored in Sect. 4 and a specific map related to the logarithm is considered. Section 5 gives more details of the two Hopf algebras of trees and their connection with the composition and substitution laws. Finally, Sect. 6 mentions an extension to P-series, which are of great use for partitioned or split systems of ordinary differential equations, and to S-series.

2 Trees, B-series, Ordered Subtrees, and Partitions

This section introduces trees, B-series, ordered subtrees and partitions of trees, concepts which are fundamental in this work. We closely follow the notation of [26, Chap. III].

2.1 Trees and B-series

Let $T = \{\bullet, [\bullet], [\bullet,\bullet], \ldots\}$ be the set of rooted trees, and let $\emptyset$ be the empty tree. For $\tau_1, \ldots, \tau_m \in T$, we denote by $\tau = [\tau_1, \ldots, \tau_m]$ the tree obtained by grafting the roots of $\tau_1, \ldots, \tau_m$ to a new vertex which becomes the root of τ. The order $|\tau|$ of a tree τ is its number of vertices and its symmetry coefficient is defined recursively by

$$\sigma(\bullet) = 1, \qquad \sigma(\tau) = \sigma(\tau_1)\cdots\sigma(\tau_m)\mu_1!\mu_2!\cdots, \tag{12}$$

where the integers $\mu_1, \mu_2, \ldots,$ count equal trees among $\tau_1, \ldots, \tau_m$. The elementary differentials $F_f(\tau)$ are given by

$$F_f(\bullet)(y) = f(y), \qquad F_f(\tau)(y) = f^{(m)}(y)\big(F_f(\tau_1)(y), \ldots, F_f(\tau_m)(y)\big).$$

For real coefficients $a(\emptyset)$ and $a(\tau)$, $\tau \in T$, a B-series is a formal series of the form

$$B(a, hf, y) = a(\emptyset)y + \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau) F_f(\tau)(y).$$

The factor $h^{|\tau|}$ is included for historical reasons and motivated by the fact that originally the most important B-series were Taylor series expansions of the exact and numerical solution. One can assume $h = 1$ because, as the notation $B(a, hf, y)$ suggests, the factor h is only a rescaling of the vector field. The normalization with the symmetry coefficient $\sigma(\tau)$ in the denominator has been proposed in [7] to give the composition law a more elegant form.

2.2 Ordered Subtrees

The general formula for the composition law needs the following notions. An ordered subtree[2] of $\tau \in T$ is a subset s of the set of all $|\tau|$ vertices which is (i) connected (by edges of the tree τ) and (ii) contains the root of τ (if s is not empty). The set of all ordered subtrees of τ is denoted by $\mathcal{S}(\tau)$. It is given in Table 1 for a tree of order 5. Associated to an ordered subtree $s \in \mathcal{S}(\tau)$ are:

- $\tau \setminus s$ is the forest (collection of rooted trees) that remains when the vertices of the subtree s together with its adjacent edges are removed from the tree τ;
- s_τ is the rooted tree given by the vertices of s with root and edges induced by that of the tree τ.

Notice that, due to the fact that we consider all vertices of τ as different, the second and third subtrees in Table 1 are different, even if s_τ and $\tau \setminus s$ are identical for both of them. This is the reason why we use the notation "ordered" subtree.

[2] Ordered subtrees are called "admissible cuts" in [18].

Table 1 All ordered subtrees of a tree with associated functions

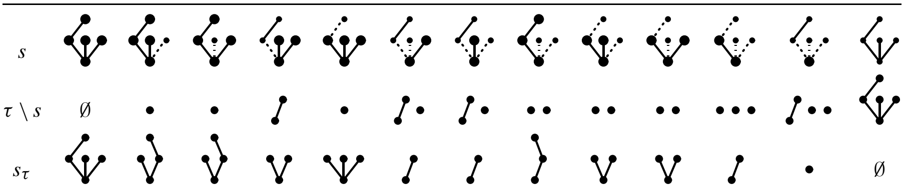
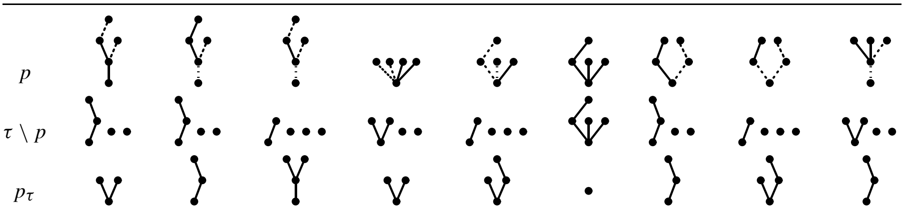


Table 2 Examples of partitions of trees with associated functions



2.3 Partitions of Trees

The substitution law needs the notation of partitions. A partition p of a tree τ is a subset of the edges of the tree. We denote by $\mathcal{P}(\tau)$ the set of all partitions p of τ (including the empty partition). Associated to such a partition are the following objects (see Table 2):

- $\tau \setminus p$ is the forest that remains when the edges of p are removed from the tree τ;
- p_τ, called *skeleton* [16], is the tree obtained by contracting each tree of $\tau \setminus p$ to a single vertex $\bullet$ and by re-establishing the edges of p.

Notice that a tree $\tau \in T$ has exactly $2^{|\tau|-1}$ partitions $p \in \mathcal{P}(\tau)$, and that different partitions may lead to the same skeleton p_τ or the same forest $\tau \setminus p$.

3 Composition and Substitution Laws

Using the notation introduced in Sect. 2 we present the general formulae for the composition and substitution laws. We also discuss their significance in the numerical treatment of differential equations.

3.1 The Composition Law

We extend[3] maps $b\colon T_0 \to \mathbb{R}$ satisfying $b(\emptyset) = 1$ to forests by putting $b(\tau_1 \dots \tau_n) := \prod_{i=1}^{n} b(\tau_i)$.

[3]This extension from trees to forests can be interpreted in the context of Hopf algebras: the extended map on the Hopf algebra Connes & Kreimer is a character, i.e. a unital algebra map (see Sect. 5 below).

Theorem 3.1 *Let $a, b\colon T_0 \to \mathbb{R}$ be two mappings, with $b(\emptyset) = 1$. Then, we have*

$$B\big(a, hf, B(b, hf, y)\big) = B(b \cdot a, hf, y),$$

where $b \cdot a\colon T_0 \to \mathbb{R}$ is defined by $(b \cdot a)(\emptyset) = a(\emptyset)$ and

$$(b \cdot a)(\tau) = \sum_{s \in \mathcal{S}(\tau)} b(\tau \setminus s) a(s_\tau). \tag{13}$$

For trees up to order 3 this formula corresponds to those of (5). The proof for a general tree τ is by Taylor series expansion and can be read in [26, Sect. III.1.4]. As mentioned in the Introduction, the set $G_C = \{a\colon T_0 \to \mathbb{R}; a(\emptyset) = 1\}$ equipped with the product (13) is a group. Associativity can be verified by algebraic manipulations, but it is also a consequence of Theorem 3.1 and the associativity of mappings. The identity element in G_C is given by

$$\delta_\emptyset(\emptyset) = 1 \quad \text{and} \quad \delta_\emptyset(\tau) = 0 \quad \text{for } \tau \in T, \tag{14}$$

which corresponds to the B-series $B(\delta_\emptyset, hf, y) = y$. The existence of an inverse follows recursively from formula (13), because for $a \in G_C$ it has the form $(b \cdot a)(\tau) = b(\tau) + a(\tau) + \cdots$, where dots indicate expressions involving trees with lower order than that of τ.

It is essential for applications that Theorem 3.1 is valid without any restrictions on $a(\emptyset)$. The most important special case of this theorem is the formula

$$hf\big(B(b, hf, y)\big) = B(b', hf, y), \tag{15}$$

where, as a consequence of the product (13), we have $b'(\emptyset) = 0$ and

$$b'(\tau) = b(\tau_1) \cdot \cdots \cdot b(\tau_m) \quad \text{for } \tau = [\tau_1, \ldots, \tau_m]. \tag{16}$$

Exact Solution of (1)

The solution $y(t+h)$ of (1) with initial value $y(t) = y$ is a B-series $y(t+h) = B(e, hf, y)$. Differentiation with respect to h shows that $h\dot{y}(t+h)$ is the B-series with coefficients $|\tau| \cdot e(\tau)$. Equating these coefficients with those of the B-series for $hf(y(t+h)) = B(e', hf, y)$ yields the recurrence relation $|\tau| \cdot e(\tau) = e(\tau_1) \cdot \cdots \cdot e(\tau_m)$.

Order Conditions for Runge–Kutta Methods

This is the origin of the consideration of B-series and of the Butcher group. A Runge–Kutta method is given by

$$g_i = y_n + h \sum_{j=1}^{s} a_{ij} f(g_j)$$

together with a similar formula for the numerical approximation y_{n+1} after one step with length h. Assuming $g_i = B(\phi_i, hf, y_n)$, the Runge–Kutta equation can be written in terms of the coefficients of the B-series as $\phi_i(\emptyset) = 1$ and, for $\tau = [\tau_1, \dots, \tau_m]$,

$$\phi_i(\tau) = \sum_{j=1}^{s} a_{ij}\,\phi'_j(\tau) = \sum_{j=1}^{s} a_{ij}\,\phi_j(\tau_1)\cdot \dots \cdot \phi_j(\tau_m).$$

These coefficients and those for the numerical approximation $y_{n+1} = B(\phi, hf, y_n)$ only depend on the parameters of the Runge–Kutta method. The order of the method, which is the largest integer p such that $y(h) - y_1 = \mathcal{O}(h^{p+1})$ for all differential equations, is now expressed by the algebraic relations $\phi(\tau) = e(\tau)$ for $|\tau| \le p$, where ϕ and e are the coefficients of the numerical and exact solution, respectively.

Effective Order

An early application of the group structure is the concept of effective order. The idea [4] is to construct a numerical method $y_{n+1} = \Phi_h(y_n)$ such that for a suitable mapping χ_h the composition $\Psi_h = \chi_h^{-1} \circ \Phi_h \circ \chi_h$ is a method of higher order. In a constant step size implementation we have $\Psi_h^n = \chi_h^{-1} \circ \Phi_h^n \circ \chi_h$, so that for the computational cost of the method Φ_h we obtain a higher accuracy by slightly modifying the initial value and by correcting the output approximation. Method Φ_h is called to be of effective order p, if Ψ_h is of order p. Assuming $\Phi_h(y) = B(a, hf, y)$ and $\chi_h(y) = B(c, hf, y)$, the conditions for effective order p are $(c \cdot a \cdot c^{-1})(\tau) = e(\tau)$ for $|\tau| \le p$, where we have employed the product (13). The mapping χ_h is called a *processor*. Notice that this notion is different from *preprocessed* (*modifying*) *vector field integrators* described in the next Sect. 3.2.

Conjugate Methods

The idea of effective order has a wide applicability in the context of geometric numerical integration. The relation $\Psi_h = \chi_h^{-1} \circ \Phi_h \circ \chi_h$ means that Φ_h and Ψ_h are conjugate maps. If Φ_h, Ψ_h, χ_h are B-series with coefficients a, b, c, respectively, then the conjugacy condition is best written in the form $(c \cdot a)(\tau) = (b \cdot c)(\tau)$, so that the composition law (13) can be directly applied. When, for some reason, a method $y_{n+1} = \Phi_h(y_n)$ cannot satisfy a desirable geometric property (like symplecticity) one can still ask whether it is conjugate to a method having this property. Extensive use of (13) has been made recently in proving conjugate-symplecticity up to order $2s + 2$ for a class of energy-preserving B-series integrators of order $2s$, see [25].

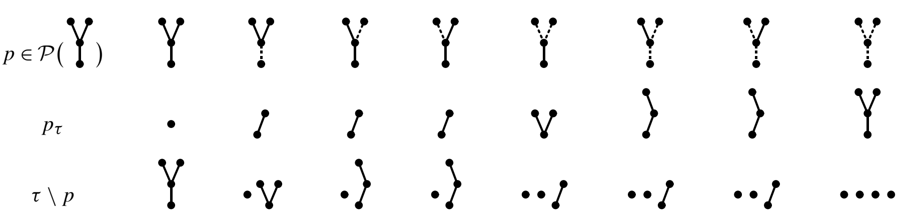
3.2 The Substitution Law

The general formula for the substitution law is as follows:

Theorem 3.2 *Let $a, b\colon T_0 \to \mathbb{R}$ be two mappings, with $b(\emptyset) = 0$. Then we have*

$$B\big(a, B(b, hf, \cdot), y\big) = B(b \star a, hf, y),$$

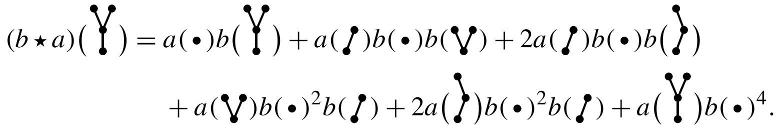
Table 3 All 8 partitions of a tree with skeletons and tree forests



where $b \star a \colon T_0 \to \mathbb{R}$ *is defined by* $(b \star a)(\emptyset) = a(\emptyset)$ *and*

$$(b \star a)(\tau) = \sum_{p \in \mathcal{P}(\tau)} b(\tau \setminus p) a(p_\tau). \tag{17}$$

For trees up to order 3 we recover the formulae (6). A detailed proof of the general case is given in [15], see also [14]. For the tree of Table 3, formula (17) yields



The set $G_S = \{a \colon T_0 \to \mathbb{R}; a(\emptyset) = 0\}$, considered in the Introduction, together with the product (17) forms a monoid. Invertible elements are those with $a(\bullet) \neq 0$ and form the group G_S^*. The identity element is $\delta_\bullet$ defined by

$$\delta_\bullet(\emptyset) = 0, \qquad \delta_\bullet(\bullet) = 1 \quad \text{and} \quad \delta_\bullet(\tau) = 0 \quad \text{for } |\tau| \geq 2. \tag{18}$$

The monoid and group properties are discussed further in Sect. 4. As we shall see in the following applications, it is important to note that Theorem 3.2 is valid without any restrictions on $a(\tau)$, e.g., also for $a \notin G_S$.

Backward Error Analysis

This is a fundamental tool for the study of the longtime behavior of geometric integrators (e.g., symplectic or reversible methods) [26, 32]. The idea is to interpret the numerical solution of a method $y_{n+1} = \Phi_h(y_n)$ applied to (1) as the exact solution of a modified differential equation $\dot{y} = f_h(y)$. For structured problems, such as Hamiltonian systems, the study of the flow of the modified differential equation gives much insight into the numerical solution.

For the case that the numerical integrator is represented by a B-series, $\Phi_h(y) = B(a, hf, y)$, it turns out that also the modified differential equation is a B-series vector field $hf_h(y) = B(b, hf, y)$ [24]. It is defined by

$$B\big(e, B(b, hf, \cdot), y\big) = B(a, hf, y),$$

where the coefficients $e(\tau)$ are those of the exact solution, given in Sect. 3.1. The coefficients of the B-series for the modified differential equation are recursively given by $(b\star e)(\tau)=a(\tau)$, because $(b\star e)(\tau)=b(\tau)+$ lower order terms.

Modifying Integrators

Modifying (or preprocessed) integrators [15] permit to increase the order of accuracy of a basic integrator $y_{n+1}=\Phi_h(y_n)$ without destroying its geometric properties. The idea is to find a modified vector field $f_h(y)$ (different from that of backward error analysis) such that the basic method applied to $\dot y=f_h(y)$ reproduces the exact solution of (1). Suitable truncation of the modified differential equation yields high order integrators. This idea has successfully been applied to the equations of motion for the rigid body [15, 28, 35].

In complete analogy to backward error analysis we have that for a B-series method $\Phi_h(y)=B(a,hf,y)$ the modified differential equation is a B-series $hf_h(y)=B(b,hf,y)$. It is defined by

$$B\big(a,B(b,hf,\cdot),y\big)=B(e,hf,y),$$

which leads to the condition $(b\star a)(\tau)=e(\tau)$ for the coefficients of the arising B-series. Again, $b(\tau)$ can be computed recursively from this relation.

Notice that the coefficients $b\in G_S^*$ for backward error analysis and modifying integrators are inverse elements with respect to the substitution law.

4 Interactions Between the Groups

We study in this section the properties and connections between the composition law and the substitution law. The proofs provided here use the interpretation in terms of B-series, and have first been given in the unpublished report [14].

4.1 A Monoid Action by Morphisms

We show that the substitution law can be seen as a monoid action of the monoid of vector fields on the Butcher group.

Theorem 4.1 *The monoid of vector fields* $(G_S,\star)$ *acts by morphisms on the Butcher group* $(G_C,\cdot)$ *via the substitution law*:

$$\begin{aligned} G_S\times G_C&\to G_C,\\ (b,a)&\mapsto b\star a. \end{aligned}$$

In particular, we have the compatibility relations

$$(b_1\star b_2)\star a=b_1\star(b_2\star a), \tag{19}$$

$$b\star(a_1\cdot a_2)=(b\star a_1)\cdot(b\star a_2), \tag{20}$$

$$(b\star a)^{-1}=b\star\big(a^{-1}\big) \tag{21}$$

for all $b,b_1,b_2\in G_S$, $a,a_1,a_2\in G_C$. *Here*, a^{-1} *denotes the inverse in* G_C.

Proof The connection of the products with B-series (Theorem 3.1 and Theorem 3.2) permits us to give simple proofs:

- (19) is a consequence of the associativity of the composition of functions, here of the form $hf \mapsto B(c, hf, y)$ for different mappings c.
- (20) means that considering the composition of the flows of two B-series $B(a_1, hf, y)$ and $B(a_2, hf, y)$, it is equivalent to substitute the vector field hf by another B-series $B(b, hf, \cdot)$ before or after the composition of the flows.
- (21) is an immediate consequence of (20), putting $a_1 = a$ and $a_2 = a^{-1}$.

A purely algebraic proof of these properties has recently been given in [8]. □

As already explained in Sect. 3.1, the coefficients $a^{-1}(\tau)$ can be computed straightforwardly by induction on $|\tau|$ from the relation $a \cdot a^{-1} = \delta_\emptyset$, and for the first trees we obtain

$$\begin{aligned} a^{-1}(\bullet) &= -a(\bullet), \\ a^{-1}([\bullet]) &= -a([\bullet]) + a(\bullet)^2, \\ a^{-1}([\bullet,\bullet]) &= -a([\bullet,\bullet]) + 2a(\bullet)a([\bullet]) - a(\bullet)^3, \\ a^{-1}([[\bullet]]) &= -a([[\bullet]]) + 2a(\bullet)a([\bullet]) - a(\bullet)^3. \end{aligned} \tag{22}$$

4.2 The Exponential and Logarithmic Maps

For a B-series method $\Phi_h(y) = B(a, hf, y)$, the coefficients b for backward error analysis are given by $b \star e = a$ (see Sect. 3.2). This relation means that the B-series $B(a, hf, y)$ is the exact flow of the differential equation with vector field $B(b, hf, y)$. Motivated by the standard notation of flows we use exponential and logarithm in place of $b \star e = a$ (see [40]),

$$a = \exp(b) \quad \text{and} \quad b = \log(a).$$

The exponential and logarithmic maps

$$\exp\colon G_S \to G_C \qquad \log\colon G_C \to G_S$$

allow us to interpret important results in geometric numerical integration in terms of one-to-one correspondences between subgroups of the Butcher group G_C and submonoids of the monoid of vector fields G_S:

- the subgroup of methods of order at least p $\{a \in G_C; a(\tau) = e(\tau) \text{ for } 1 \le |\tau| \le p\}$ corresponds to the submonoid $\{b \in G_S; b(\bullet) = 1, b(\tau) = 0 \text{ for } 2 \le |\tau| \le p\}$;
- the subgroup of symmetric B-series methods $\{a \in G_C;\ B(a^{-1}, hf, y) = B(a, -hf, y)\}$ is in correspondence with the submonoid $\{b \in G_S;\ b(\tau) = 0$ for $|\tau|$ even$\}$;
- the subgroup of symplectic B-series methods characterized by [9]

$$\big\{a \in G_C; a(u \circ v) + a(v \circ u) = a(u)a(v) \text{ for } u, v \in T\big\}$$

corresponds to the submonoid of Hamiltonian vector fields characterized by [24]

$$\{b \in G_S; b(u \circ v) + b(v \circ u) = 0 \text{ for } u, v \in T\},$$

where $u \circ v := [u_1, \dots, u_n, v]$ for $u = [u_1, \dots, u_n], v \in T$ denotes the Butcher product, see [26, Def. III.3.7];
- the subgroup of energy-preserving B-series methods in G_C is in correspondence with the submonoid of vector fields in G_S having the energy as first integral.
- the subgroup of volume-preserving methods in G_C is in correspondence with the submonoid of divergence-free vector fields in G_S. Theses classes of B-series integrators and vector fields were studied recently in [17, 31].

Proofs of these statements are given in Theorems IX.1.2, IX.2.2, IX.3.1, and Corollaries IX.5.4, IX.9.13 of [26]. It is interesting to note that geometric properties are non-linear conditions in G_C and become linear in G_S.

4.3 The Special Role of the Explicit Euler Method

Consider the explicit Euler method

$$y_{n+1} = y_n + hf(y_n) \tag{23}$$

which is the simplest B-series integrator, with coefficients $\delta_\emptyset + \delta_\bullet$, see definitions (14) and (18). We denote by

$$\omega := \log(\delta_\emptyset + \delta_\bullet) \tag{24}$$

the coefficients of its modified vector field for backward error analysis.

Theorem 4.2 *The inverse of a in the Butcher group G_C is given explicitly by*

$$a^{-1} = (a - \delta_\emptyset) \star (\delta_\emptyset + \delta_\bullet)^{-1} \tag{25}$$

and coefficients for backward error analysis are obtained explicitly in terms of ω by

$$\log(a) = (a - \delta_\emptyset) \star \omega. \tag{26}$$

Proof Any B-series integrator $y_{n+1} = B(a, hf, y_n)$ can be interpreted as the explicit Euler method (23), where the vector field hf is replaced by the B-series vector field with coefficients $a - \delta_\emptyset$, which yields $a = (a - \delta_\emptyset) \star (\delta_\emptyset + \delta_\bullet)$. Then, application of property (21) yields relation (25).

Coefficients ω are defined by $\omega \star e = \delta_\emptyset + \delta_\bullet$. Subtracting $\delta_\emptyset$ on both sides we obtain $\omega \star (e - \delta_\emptyset) = \delta_\bullet$, which means that $\omega = (e - \delta_\emptyset)^{\star -1}$ is the inverse for the substitution law of the exact solution. Now, $\log(a)$ is defined by $\log(a) \star e = a$. Subtracting $\delta_\emptyset$ on both sides, and multiplying by ω from the right side yields the statement (26). □

Explicit Formula for the Inverse in the Butcher Group

Since for $a = \delta_\emptyset + \delta_\bullet$ only two terms are non-zero in (13), we get by induction on $|\tau|$ that $(\delta_\emptyset + \delta_\bullet)^{-1}(\tau) = (-1)^{|\tau|}$. Using the general formula (17) for the substitution law, formula (25) allows to recover the following formula for the inverse of an element a in G_C, a result first discovered in [18] in the context of Hopf algebras of trees:

$$a^{-1}(\tau) = \sum_{p\in\mathcal{P}(\tau)} (-1)^{|p_\tau|} a(\tau \setminus p). \tag{27}$$

For trees up to order 3 this formula yields again (22).

Explicit Formula for the Logarithmic Map

Once the coefficients $\omega(\tau)$ are tabulated (see Table 4 for trees up to order 5), (26) together with (17) give an explicit formula for the logarithm $\log(a)$ of backward error analysis. In the context of combinatorial Hopf algebras the coefficients ω can be traced back to [11] under the name $\log^*$ and are studied also in [8, 12, 22, 40].

The coefficients $\omega(\tau)$ may be computed by induction from the relation $\omega \star e = \delta_\emptyset + \delta_\bullet$ using formula (17). The coefficients $\omega(\tau)$ for the bushy trees , , , ... are the Bernoulli numbers B_i. They correspond to quadrature problems $\dot{y} = f(t)$, see [26, Example IX.7.1],

$\omega($$) = B_1 = -1/2,$ $\omega($$) = B_2 = 1/6,$

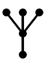
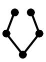
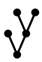
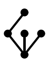
$\omega($$) = B_3 = 0,$ $\omega($$) = B_4, \ldots.$

Coefficients for tall trees $\bullet$, , , ... correspond to linear problems $\dot{y} = \lambda y$, and are simply those of the series of $\log(1+x)$:

$\omega(\bullet) = 1,$ $\omega($$) = -1/2,$ $\omega($$) = 1/3,$

$\omega($$) = -1/4,$ $\omega($$) = 1/5, \ldots.$

Table 4 Coefficients $\omega(\tau)$ for trees of order ≤ 5

τ	$\emptyset$	$\bullet$							
$\omega(\tau)$	0	1	$-\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{3}$	0	$-\frac{1}{6}$	$-\frac{1}{4}$	$-\frac{1}{12}$
τ									
$\omega(\tau)$	$-\frac{1}{30}$	$\frac{1}{30}$	$\frac{1}{5}$	$\frac{1}{20}$	$\frac{1}{30}$	$\frac{3}{20}$	$\frac{1}{60}$	$-\frac{1}{60}$	$\frac{1}{10}$

Proposition 4.3 *The coefficients ω satisfy the following relation for all $u, v \in T$,*

$$\omega(u \circ v) + \omega(v \circ u) + \omega(u \times v) = 0. \tag{28}$$

This generalizes to three trees (and more),

$$\omega\big(u \circ (vw)\big) + \omega\big(v \circ (wu)\big) + \omega\big(w \circ (uv)\big) + \omega\big((u \times v) \circ w\big) + \omega\big((v \times w) \circ u\big) + \omega\big((w \times u) \circ v\big) + \omega(u \times v \times w) = 0. \tag{29}$$

Moreover, ω is the unique mapping of G_S satisfying both $\omega(\bullet) = 1$ and (28)–(29).

Here, $\circ$ and $\times$ denote respectively the *Butcher* product and the *merging* product,

$$u \circ (vw \ldots) = [u_1, \ldots u_n, v, w \ldots], \qquad u \times v \times \cdots = [u_1, \ldots u_n, v_1 \ldots v_m, \ldots],$$

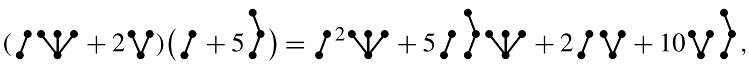
for all trees $u = [u_1, \ldots u_n]$, $v = [v_1, \ldots v_m]$, $w, \ldots$. A direct proof of (28)–(29) is obtained using the substitution law formula in [14, Prop. 4.4]. An algebraic proof using quasi-shuffle products is given in [8, Sect. 9]. The uniqueness of ω is a consequence of results in [13], where it is shown that among B-series methods, only the (time-scaled) exact flow conserves both quadratic and cubic invariants, i.e., satisfies

$$e(u \circ v) + e(v \circ u) = e(u)e(v),$$
$$e\big(u \circ (vw)\big) + e\big(v \circ (wu)\big) + e\big(w \circ (uv)\big) = e(u)e(v)e(w).$$

5 Two Hopf Algebras of Trees

There is a close connection between the results of the previous sections and Hopf algebras of trees. The composition law is related to a Hopf algebra introduced by Connes, Kreimer and Moscovici [18–20] (see the review [34]), whereas the substitution law is related to a Hopf algebra introduced by Calaque et al. [8].

We consider the set $\mathcal{H}$ of linear combinations of forests of rooted trees. As for standard polynomials we consider scalar multiplication, addition and multiplication which makes this set a commutative algebra. For example, the product of two polynomials is



and the identity element for the multiplication is the empty tree $e = \emptyset$. Such an algebra equipped with a coproduct $\Delta\colon \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$, which is coassociative,

$$(Id \otimes \Delta) \circ \Delta = (\Delta \otimes Id) \circ \Delta, \tag{30}$$

and compatible with the algebra laws is called a bialgebra. It is a Hopf algebra if in addition it is equipped with an antipode $S\colon \mathcal{H} \to \mathcal{H}$ which is an algebra map[4]

[4]In general, the antipode is an algebra antimorphism: $S(u)S(v) = S(vu)$. If the Hopf algebra is commutative, it reduces to an algebra map. This is the case here, but not in [33, 38] in the context of Lie group integrators.

satisfying

$$\mu \circ (S \otimes Id) \circ \Delta = \mu \circ (Id \otimes S) \circ \Delta = e\delta_e \tag{31}$$

where $\mu\colon \mathcal{H} \otimes \mathcal{H} \to \mathcal{H}$ is the multiplication of elements in $\mathcal{H}$.

5.1 The Hopf Algebra of Connes & Kreimer

Let us consider the commutative $\mathbb{R}$-algebra of polynomials on trees T_0 (including the empty tree). We recall that elements a in the Butcher group G_C satisfy $a(\emptyset) = 1$ and can be extended to unital algebra maps by $a(\tau_1 \dots \tau_n) = a(\tau_1) \cdots (\tau_n)$ and by linearity.

According to [18–20] we define the coproduct $\Delta_{CK}\colon \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$ on trees,

$$\Delta_{\mathrm{CK}}(\tau) = \sum_{s \in \mathcal{S}(\tau)} (\tau \setminus s) \otimes s_\tau,$$

and we extend Δ_{CK} to an unital algebra map. There is a striking similarity [2, 3] with formula (13) for the composition law of the Butcher group. Indeed, if we apply b on the left side of the tensor product and a on the right side, we obtain $(b \cdot a)(\tau)$. This connection can be expressed by the formula

$$(b \cdot a)(\tau) = \bigl(\mu \circ (b \otimes a) \circ \Delta_{\mathrm{CK}}\bigr)(\tau), \tag{32}$$

where $\mu\colon \mathbb{R} \otimes \mathbb{R} \to \mathbb{R}$ denotes the multiplication. In the context of combinatorial Hopf algebra, this is called a convolution product. We say that the Butcher group corresponds to the group of characters of the Hopf tree algebra of Connes & Kreimer.

The validity of (30) can be understood as follows: by definition of the coproduct, we have

$$\bigl((Id \otimes \Delta_{\mathrm{CK}}) \circ \Delta_{\mathrm{CK}}\bigr)(\tau) = \sum_{s \in \mathcal{S}(\tau)} \sum_{s' \in \mathcal{S}(s_\tau)} (\tau \setminus s) \otimes (s_\tau \setminus s') \otimes s'_\tau$$

and for the composition law we have

$$\bigl(a \cdot (b \cdot c)\bigr)(\tau) = \sum_{s \in \mathcal{S}(\tau)} \sum_{s' \in \mathcal{S}(s_\tau)} a(\tau \setminus s)\, b(s_\tau \setminus s')\, c(s'_\tau).$$

Similar formulae for the right side of (30) together with the associativity $a \cdot (b \cdot c) = (a \cdot b) \cdot c$ in the Butcher group prove the coassociativity property (30) for Δ_{CK}.

The antipode $S_{\mathrm{CK}}\colon \mathcal{H} \to \mathcal{H}$ is given by

$$S_{\mathrm{CK}}(\tau) = \sum_{p \in \mathcal{P}(\tau)} (-1)^{|p_\tau|} (\tau \setminus p),$$

which yields for the first trees,

$$S_{\mathrm{CK}}(\emptyset) = \emptyset,$$

$$S_{\mathrm{CK}}(\bullet) = -\bullet,$$

$$S_{\mathrm{CK}}([\bullet]) = -[\bullet] + \bullet^2,$$

$$S_{\mathrm{CK}}([\bullet,\bullet]) = -[\bullet,\bullet] + 2\bullet[\bullet] - \bullet^3,$$

$$S_{\mathrm{CK}}([[\bullet]]) = -[[\bullet]] + 2\bullet[\bullet] - \bullet^3.$$

Again, there is a strong similarity with the Butcher group, compare with formulae (22) and (27): the inverse in the Butcher group is related to the antipode S_{CK} by

$$a^{-1}(\tau) = (a \circ S_{\mathrm{CK}})(\tau).$$

This can be seen from (31) and (32) which yield $a \cdot (a \circ S_{\mathrm{CK}}) = (a \circ S_{\mathrm{CK}}) \cdot a = \delta_\emptyset$.

5.2 A Bialgebra Based on the Substitution Law

In the recent article [8] a Hopf algebra of trees has been constructed, with a new coproduct that is closely related to the substitution law (17). For the same algebra as in Sect. 5.1, we consider here the coproduct (see (11))

$$\Delta_{\mathrm{CEM}}(\tau) = \sum_{p \in \mathcal{P}(\tau)} (\tau \setminus p) \otimes p_\tau. \tag{33}$$

which is slightly different from that of [8], cf. Sect. 5.3.

In analogy to the relation between the coproduct of Connes & Kreimer and the composition law, the convolution product for the coproduct (33) is exactly the substitution law of (17). For $a, b \in G_S$, we have

$$(b \star a)(\tau) = \big(\mu \circ (b \otimes a) \circ \Delta_{\mathrm{CEM}}\big)(\tau).$$

The coassociativity of Δ_{CEM} follows as in Sect. 5.1. We thus get a bialgebra.[5] Since G_S is a monoid but not a group, it is not surprising that no antipode associated to this coproduct exists.

5.3 The Hopf Algebra of Calaque, Ebrahimi-Fard & Manchon

In the article [8] it is shown how the algebra $\mathcal{H}$ has to be modified so that the coproduct Δ_{CEM} of (33) gives rise to a Hopf algebra structure.

We let $\mathcal{H}_{\mathrm{CEM}}$ be the commutative $\mathbb{R}$-algebra of polynomials on trees T (excluding the empty tree), with $e = \bullet$ as the identity element (in contrast to the algebra of Sects. 5.1 and 5.2). We equip this algebra with the coproduct Δ_{CEM} of (33). Since $\bullet$ is the identity element, it can be removed when multiplied with other trees. For example, we have

$$\Delta_{\mathrm{CEM}}([[\bullet]]) = [[\bullet]] \otimes \bullet + 2[\bullet] \otimes [\bullet] + \bullet \otimes [[\bullet]]$$

[5] In a private communication, Dominique Manchon pointed out that $\mathcal{H}$ equipped with the coproduct Δ_{CEM} is a bialgebra which is graded but not connected. In fact, a graded bialgebra which is connected is automatically a Hopf algebra, i.e. an antipode exists.

which should be compared to (11). In the context of B-series, the choice $e = \bullet$ for the identity element corresponds to the subgroup of G_S

$$G_S^1 = \{a\colon T \to \mathbb{R};\, a(\bullet) = 1\},$$

which corresponds to B-series vector fields of the form $hf(y)$ + higher order terms. The inverse $a^{\star-1}(\tau)$ of $a \in G_S^1$ (with respect to the substitution law) can be computed recursively from (17). For trees up to order 3 we obtain

$$\begin{aligned}
a^{\star-1}(\bullet) &= a(\bullet) = 1, & S_{\mathrm{CEM}}(\bullet) &= \bullet,\\
a^{\star-1}([\bullet]) &= -a([\bullet]), & S_{\mathrm{CEM}}([\bullet]) &= -[\bullet],\\
a^{\star-1}([\bullet,\bullet]) &= -a([\bullet,\bullet]) + 2a([\bullet])^2, & S_{\mathrm{CEM}}([\bullet,\bullet]) &= -[\bullet,\bullet] + 2[\bullet]^2,\\
a^{\star-1}([[\bullet]]) &= -a([[\bullet]]) + 2a([\bullet])^2, & S_{\mathrm{CEM}}([[\bullet]]) &= -[[\bullet]] + 2[\bullet]^2.
\end{aligned} \tag{34}$$

This readily permits us to define an antipode by the formulas to the right of (34), which makes the bialgebra a Hopf algebra. A general formula for this antipode is given in [8]. Since it requires additional notations, we do not reproduce it here. Similarly to the relation between G_C and $\mathcal{H}_{\mathrm{CK}}$ (Sect. 5.1), the group G_S^1 corresponds to the group of characters of the Hopf algebra $\mathcal{H}_{\mathrm{CEM}}$.

6 Extensions

There exist many different extensions of B-series in the numerical analysis literature, e.g., P-series [23] for partitioned differential equations, DAE-series for differential-algebraic equations, Lie–Butcher series [37], S-series [39] and LS-series [38] for differential operators. We briefly present the ideas of P-series and S-series.

6.1 P-series

Partitioned systems of differential equations

$$\dot p = f^{[1]}(p,q), \qquad \dot q = f^{[2]}(p,q)$$

arise in many situations. Second-order differential equations when written in first-order form and Hamiltonian systems are interesting special cases. There are important numerical integrators that treat the variables p and q in a different manner, e.g., symplectic methods based on the Störmer–Verlet integrator [26]. P-series are an extension of B-series adapted to partitioned systems [27, Sect. II.15].

Let $TP_0 = \{\emptyset_p, \emptyset_q, \bullet, \circ, [\bullet]_\bullet, [\circ]_\circ, [\bullet]_\circ, \dots\}$ denote the set of bi-colored trees, and $\emptyset_p, \emptyset_q$ denote empty trees. For a mapping $a : TP_0 \to \mathbb{R}$ a P-series is of the form

$$\begin{aligned}
P(a, hf, y) &= \begin{pmatrix} a(\emptyset_p)p \\ a(\emptyset_q)q \end{pmatrix} + h \begin{pmatrix} a(\bullet) f^{[1]} \\ a(\circ) f^{[2]} \end{pmatrix}\\
&\quad + h^2 \begin{pmatrix} a([\bullet]_\bullet)(f_p^{[1]} f^{[1]}) + a([\circ]_\bullet)(f_q^{[1]} f^{[2]}) \\ a([\bullet]_\circ)(f_p^{[2]} f^{[1]}) + a([\circ]_\circ)(f_q^{[2]} f^{[2]}) \end{pmatrix} + \cdots,
\end{aligned}$$

with functions evaluated at $y = (p, q)$. The upper component contains terms corresponding to trees with black root, and the lower component to trees with white root.

Results for B-series of previous sections can be extended straight-forwardly to P-series. We again have a composition law

$$P\big(a, hf, P(b, hf, y)\big) = P(b \cdot a, f, y)$$

and a substitution law

$$P\big(a, P(b, hf, \cdot), y\big) = P(b \star a, f, y).$$

The formulas of Theorem 3.1 and Theorem 3.2 are still valid, where trees, subtrees, and skeletons are now in TP_0. The only ambiguity that could arise is in the definition of the skeleton p_τ: the color of a vertex of p_τ is that of the root of the tree which is replaced by the vertex.

For instance, for the partition $p =$ we have $p_\tau =$. An example for the substitution law is

$$(b \star a)(\;) = a(\bullet)b(\;) + a(\;)b(\bullet)b(\;) + a(\;)b(\circ)b(\;) + a(\;)b(\bullet)^2 b(\circ).$$

6.2 S-series

S-series have been introduced by Murua [39] for the purpose of analyzing the preservation of invariants, either in the context of differential-algebraic equations or in the context of Hamiltonian dynamics. If g is a first integral of (1), i.e., $g'(y)f(y) \equiv 0$, it is natural to investigate whether the numerical approximation $y_{n+1} = B(a, hf, y_n)$ provided by a B-series method satisfies $g(y_{n+1}) = g(y_n)$. This leads to the study of $g\big(B(a, hf, y)\big)$ and motivates the following definitions.

Let $g(y)$ be a scalar- or vector-valued smooth function and $f(y)$ the vector field of the system (1). We let

$$F_{g,f}(\bullet)(y) = g(y), \qquad F_{g,f}(\tau)(y) = g^{(m)}(y)\big(F_f(\tau_1)(y), \ldots, F_f(\tau_m)(y)\big), \quad (35)$$

where $\tau = [\tau_1, \ldots, \tau_m]$ and $F_f(\tau)(y)$ are the elementary differentials of Sect. 2.1. For real coefficients $a(\tau)$, $\tau \in T$, an S-series is a formal series of the form

$$S(a, hg, hf, y) = \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} a(t) F_{g,f}(\tau)(y). \quad (36)$$

For $g = f$ we recover B-series vector fields. For $g = Id$, we obtain

$$S(a, h\,Id, hf, y) = h\,B(\widehat{a}, hf, y)$$

with $\widehat{a}(\tau) = a([\tau])$ for $\tau \in T_0$, and we see that all B-series can be interpreted as S-series.

Such a series (36) can be seen as a formal linear differential operator acting on g (notice that $g \mapsto F_{g,f}(y)$ is a linear differential operator). In the original[6] literature [39, 40] on S-series and also in the context of Lie theory [33, 38] (where S-series correspond to "pullback series"), this interpretation as differential operator is very important. Indeed, for a given flow $\varphi_t(y)$ of a vector field $f(y)$ on a differentiable manifold $\mathcal{M}$, the "Vertauschungssatz" [26, p. 88] in the theory of Lie-series allows to interpret $g(\varphi_t(y))$ as a differential operator,

$$g \circ \varphi_t = \exp(tF)[g] \tag{37}$$

where $F(y) = \sum_{j=1}^{n} f_j(y) \frac{\partial}{\partial y_j}$ (here for the special case $\mathcal{M} = \mathbb{R}^n$) is the differential operator (Lie derivative) associated to the vector field $f(y)$.

There are now three possibilities of defining composition or substitution laws. One can substitute in (36) a B-series with $b(\emptyset) = 1$ for y, a B-series with $b(\emptyset) = 0$ for hf, and finally an arbitrary S-series for hg. All of these operations lead to S-series which we denote as follows:

$$S(b \cdot a, hg, hf, y) = S\big(a, hg, hf, B(b, hf, y)\big), \tag{38}$$

$$S(b \star a, hg, hf, y) = S\big(a, hg, B(b, hf, \cdot), y\big), \tag{39}$$

$$S(b * a, hg, hf, y) = S\big(a, S(b, hg, hf, \cdot), hf, y\big). \tag{40}$$

The proof of Theorem 3.1 shows that the product $(b \cdot a)(\tau)$ in (38) is given by

$$(b \cdot a)(\tau) = \sum_{s \in \mathcal{S}_0(\tau)} b(\tau \setminus s) a(s_\tau), \tag{41}$$

where $\mathcal{S}_0(\tau)$ is the set of non-empty, ordered subtrees of τ. Notice that the empty tree is not involved in the S-series (36).

The product $(b \star a)(\tau)$ in (39) is closely related to the substitution law of Theorem 3.2. The difference is that in the S-series only the function f is substituted with a B-series and the function g (corresponding to the root) is not touched. We therefore obtain the formula

$$(b \star a)(\tau) = \sum_{p \in \mathcal{P}_0(\tau)} b\big(\{\tau \setminus p\}_0\big) a(p_\tau),$$

where the sum is only over those partitions of τ which contain all edges leaving the root of τ (the set of such partitions is denoted by $\mathcal{P}_0(\tau)$), and where $\{\tau \setminus p\}_0$ is the forest obtained by removing the edges of p and also the root of τ.

The product $(b * a)(\tau)$ in (40) is given by

$$(b * a)(\tau) = \sum_{s \in \mathcal{S}_0(\tau)} b(s_\tau) a\big([\tau \setminus s]\big), \tag{42}$$

[6]In this article, we have changed the notation because it is more convenient in our context to consider g and f on the same level.

where $[\tau \setminus s]$ is the tree obtained from τ by contracting the subtree s_τ to a single vertex, which becomes the root of $[\tau \setminus s]$. All proofs are very similar to those for B-series.

Putting $a = \delta_\bullet$ in (38), we get in analogy to (15) that

$$hg\big(B(b, hf, y)\big) = S(b', hg, hf, y) \tag{43}$$

with $b'(\tau)$ given by (16). This relation is at the origin of considering S-series as mentioned in the beginning of this section. It is related to (37) and expresses in terms of S-series the exponential of the Lie derivative corresponding to the vector field $B(\log b, hf, y)$. Furthermore, replacing hg in (43) by an S-series with general coefficients $a(\tau)$ we obtain the relation

$$b \cdot a = a * b'$$

which links the products (41) and (42).

Similarly to the case of B-series, the substitution law for S-series (42) can be turned into a coproduct on the algebra of Sect. 5.3 (excluding the empty tree)

$$\Delta(\tau) = \sum_{s \in \mathcal{S}_0(\tau)} s_\tau \otimes [\tau \setminus s]$$

which yields again a Hopf algebra of trees.

Acknowledgements The authors are grateful to Damien Calaque and Dominique Manchon for helpful discussions and comments. This work was partially supported by the Fonds National Suisse, project No. 200020-109158.

References

1. S. Blanes, F. Casas, J. Ros, Symplectic integrators with processing: a general study, *SIAM J. Sci. Comput.* **21**, 149–161 (1999).
2. Ch. Brouder, Runge–Kutta methods and renormalization, *Eur. Phys. J. C* **12**, 521–534 (2000).
3. Ch. Brouder, Trees, renormalization and differential equations, *BIT* **44**(3), 425–438 (2004).
4. J.C. Butcher, The effective order of Runge–Kutta methods, in *Proceedings of Conference on the Numerical Solution of Differential Equations*, ed. by J.Ll. Morris, Lecture Notes in Math., vol. 109 (Springer, Berlin, 1969), pp. 133–139.
5. J.C. Butcher, An algebraic theory of integration methods, *Math. Comput.* **26**, 79–106 (1972).
6. J.C. Butcher, *Numerical Methods for Ordinary Differential Equations*, 2nd edn. (John Wiley & Sons Ltd., Chichester, 2008).
7. J.C. Butcher, J.M. Sanz-Serna, The number of conditions for a Runge–Kutta method to have effective order p, *Appl. Numer. Math.* **22**, 103–111 (1996).
8. D. Calaque, K. Ebrahimi-Fard, D. Manchon, Two interacting Hopf algebras of trees, *Adv. Appl. Math.* (2009, in press).
9. M.P. Calvo, J.M. Sanz-Serna, Canonical B-series, *Numer. Math.* **67**, 161–175 (1994).
10. A. Cayley, On the theory of the analytic forms called trees, *Philos. Mag.* **XIII**, 172–176 (1857).
11. F. Chapoton, Rooted trees and an exponential-like series (2002). arXiv:math/0209104.
12. F. Chapoton, A rooted-trees q-series lifting a one-parameter family of Lie idempotents, *Algebra & Number Theory* **3**(6), 611–636 (2009).
13. P. Chartier, E. Faou, A. Murua, An algebraic approach to invariant preserving integrators: the case of quadratic and Hamiltonian invariants, *Numer. Math.* **103**, 575–590 (2006).

14. P. Chartier, E. Hairer, G. Vilmart, A substitution law for B-series vector fields, INRIA Report, No. 5498 (2005).
15. P. Chartier, E. Hairer, G. Vilmart, Numerical integrators based on modified differential equations, *Math. Comput.* **76**, 1941–1953 (2007).
16. P. Chartier, E. Lapôtre, Reversible B-series. INRIA Report, No. 1221 (1998).
17. P. Chartier, A. Murua, Preserving first integrals and volume forms of additively split systems, *IMA J. Numer. Anal.* **27**(2), 381–405 (2007).
18. A. Connes, D. Kreimer, Hopf algebras, renormalization and noncommutative geometry, *Commun. Math. Phys.* **199**(1), 203–242 (1998).
19. A. Connes, D. Kreimer, Renormalization in quantum field theory and the Riemann–Hilbert problem. I. The Hopf algebra structure of graphs and the main theorem, *Commun. Math. Phys.* **210**(1), 249–273 (2000).
20. A. Connes, H. Moscovici, Hopf algebras, cyclic cohomology and the transverse index theorem, *Commun. Math. Phys.* **198**(1), 199–246 (1998).
21. A. Dür, *Möbius Functions, Incidence Algebras and Power Series Representations*. Lecture Notes in Math., vol. 1202 (Springer, Berlin, 1986).
22. K. Ebrahimi-Fard, D. Manchon, A Magnus and Fer-type formula in dendriform algebras, *Found. Comput. Math.* **9**(3), 295–316 (2009).
23. E. Hairer, Order conditions for numerical methods for partitioned ordinary differential equations, *Numer. Math.* **36**(4), 431–445 (1980/81).
24. E. Hairer, Backward analysis of numerical integrators and symplectic methods, *Ann. Numer. Math.* **1**, 107–132 (1994).
25. E. Hairer, Energy-preserving variant of collocation methods (2009, submitted for publication).
26. E. Hairer, C. Lubich, G. Wanner, *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*, 2nd edn., Springer Series in Computational Mathematics, vol. 31 (Springer, Berlin, 2006).
27. E. Hairer, S.P. Nørsett, G. Wanner, *Solving Ordinary Differential Equations I. Nonstiff Problems*, 2nd edn., Springer Series in Computational Mathematics, vol. 8 (Springer, Berlin, 1993).
28. E. Hairer, G. Vilmart, Preprocessed discrete Moser–Veselov algorithm for the full dynamics of the rigid body, *J. Phys. A* **39**, 13225–13235 (2006).
29. E. Hairer, G. Wanner, On the Butcher group and general multi-value methods, *Computing* **13**, 1–15 (1974).
30. E. Hairer, G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*, 2nd edn., Springer Series in Computational Mathematics, vol. 14 (Springer, Berlin, 1996).
31. A. Iserles, G.R.W. Quispel, P.S.P. Tse, B-series methods cannot be volume-preserving, *BIT* **47**(2), 351–378 (2007).
32. B. Leimkuhler, S. Reich, *Simulating Hamiltonian Dynamics*, Cambridge Monographs on Applied and Computational Mathematics, vol. 14 (Cambridge University Press, Cambridge, 2004).
33. A. Lundervold, H. Munthe-Kaas, Hopf algebras of formal diffeomorphisms and numerical integration on manifolds (2009, submitted). arXiv:0905.0087.
34. D. Manchon, Hopf algebras and renormalisation, in *Handbook of Algebra*, vol. 5 (Elsevier, Amsterdam, 2008), pp. 365–427.
35. R.I. McLachlan, A. Zanna, The discrete Moser–Veselov algorithm for the free rigid body, revisited, *Found. Comput. Math.* **5**, 87–123 (2005).
36. R.H. Merson, An operational method for the study of integration processes, in *Proc. Symp. Data Processing Weapons Research Establishment*, pp. 110-1–110-25, Salisbury, Australia (1957).
37. H. Munthe-Kaas, Lie Butcher theory for Runge–Kutta methods, *BIT* **35**, 572–587 (1995).
38. H. Munthe-Kaas, W. Wright, On the Hopf algebraic structure of Lie group integrators, *Found. Comput. Math.* **8**(2), 227–257 (2008).
39. A. Murua, Formal series and numerical integrators. I. Systems of ODEs and symplectic integrators, *Appl. Numer. Math.* **29**(2), 221–251 (1999).
40. A. Murua, The Hopf algebra of rooted trees, free Lie algebras, and Lie series, *Found. Comput. Math.* **6**(4), 387–426 (2006).