A substitution law for B-series vector fields

Philippe Chartier, Ernst Hairer, Gilles Vilmart

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

A substitution law for B-series vector fields

Philippe Chartier — Ernst Hairer — Gilles Vilmart

N° 5498

February 2005

THÈME 4

Rapport de recherche

ISSN 0249-6399 ISRN INRIA/RR--5498--FR+ENG

A substitution law for B-series vector fields

Philippe Chartier * , Ernst Hairer † , Gilles Vilmart ‡

Thème 4 — Simulation et optimisation
de systèmes complexes
Projet Ipso

Rapport de recherche n° 5498 — February 2005 — 24 pages

Abstract: In this paper, we derive a new composition law obtained by substituting a B-series into the vector field appearing in another B-series. We derive explicit formulas for the computation of this law and study its algebraic properties. We then focus on the specific case of Hamiltonian vector fields. It is shown that this new law allows a convenient derivation of the modified equation occurring in backward error analysis or in numerical methods based on generating functions.

Key-words: ordinary differential equations, B-series, backward error analysis, Hamiltonian, symplectic, symmetric, generating function methods

* IPSO, INRIA Rennes, France, email: `Philippe.Chartier@inria.fr`
† Dépt. de Mathématiques, Université de Genève, Switzerland, email: `Ernst.Hairer@math.unige.ch`
‡ Dépt. de Mathématiques, ENS de Cachan Bretagne, France.

Unité de recherche INRIA Rennes
IRISA, Campus universitaire de Beaulieu, 35042 Rennes Cedex (France)
Téléphone : +33 2 99 84 71 00 —Télécopie : +33 2 99 84 71 71

Une loi de substitution pour les B-séries

Résumé : Dans cet article, nous introduisons une nouvelle loi de composition des B-séries obtenue en substituant au champ de vecteur une B-série dans une autre B-séries. Une formule explicite de calcul est proposée et les propriétés algébriques de cette loi sont étudiées. Le cas hamiltonien est envisagé de manière plus spécifique.

Mots-clés : équations différentielles ordinaires, B-séries, analyse rétrograde, hamiltonien, symplectique, symétrique, fonctions génératrices

1 Introduction

Symplectic numerical schemes as proposed by Feng Kang [Fen86], Feng Kang, Wu, Qin & Wang [FWQW89] and Channel & Scovel [CS90] rely on the construction of an approximate solution of the Hamilton-Jacobi equation (see [HLW02]). For general ordinary differential equations (not necessarily Hamiltonian) of the form

$$\left\{ \begin{array}{rcl} \dot{y} & = & f(y) \\ y(0) & = & y_0 \end{array} \right. , \tag{1}$$

this idea comes to computing the first coefficients of a *modified* equation. For instance, considering the midpoint rule

$$\begin{aligned} y_1 &= y_0 + hf\Big(\frac{y_1+y_0}{2}\Big) \\ &= y_0 + hf(y_0) + \frac{h^2}{2}f'(y_0)f(y_0) + h^3\Big(\frac{1}{4}f'(y_0)f'(y_0)f(y_0) + \frac{1}{8}f''(y_0)(f(y_0),f(y_0))\Big) + \dots \end{aligned} \tag{2}$$

we search for a h-dependent modified field of the form $\breve{f}(y) = f(y) + hf_2(y) + h^2 f_3(y) + h^3 f_4(y) + \dots$ such that $\breve{y}_1$ as given by (2) with f replaced by $\breve{f}$ and y_1 by $\breve{y}_1$

$$\breve{y}_1 = y_0 + h\breve{f}\Big(\frac{\breve{y}_1+y_0}{2}\Big) \tag{3}$$

coincide with the exact solution of (1) in the sense that $y(h) = \breve{y}_1$. Expanding both terms into Taylor series

$$\begin{aligned} y(h) &= y_0 + hf(y_0) + \frac{h^2}{2}f'(y_0)f(y_0) + \frac{h^3}{6}\Big(f'(y_0)f'(y_0)f(y_0) + f''(y_0)(f(y_0),f(y_0))\Big) + \dots, \\ \breve{y}_1 &= y_0 + h\breve{f}(y_0) + \frac{h^2}{2}\breve{f}'(y_0)\breve{f}(y_0) + h^3\Big(\frac{1}{4}\breve{f}'(y_0)\breve{f}'(y_0)\breve{f}(y_0) + \frac{1}{8}\breve{f}''(y_0)(\breve{f}(y_0),\breve{f}(y_0))\Big) + \dots \\ &= y_0 + hf(y_0) + \frac{h^2}{2}\Big(f'(y_0)f(y_0) + 2f_2(y_0)\Big) + \\ &\quad h^3\Big(\frac{1}{4}\breve{f}'(y_0)\breve{f}'(y_0)\breve{f}(y_0) + \frac{1}{8}\breve{f}''(y_0)(\breve{f}(y_0),\breve{f}(y_0)) + f_3(y_0) + \frac{1}{2}f'(y_0)f_2(y_0) + \frac{1}{2}f_2'(y_0)f(y_0)\Big) + \dots, \end{aligned} \tag{4}$$

and identifying equal powers of h gives

$$\begin{aligned} f_2(y) &= 0, \\ f_3(y) &= -\frac{1}{12}f'(y)f'(y)f(y) + \frac{1}{24}f''(y)(f(y),f(y)), \\ f_4(y) &= 0, \\ \dots & \dots \dots \end{aligned}$$

Solving equation

$$\dot{y} = f(y) - \frac{h^2}{12}f'(y)f'(y)f(y) + \frac{h^2}{24}f''(y)(f(y),f(y)) + \dots, \tag{5}$$

truncated after second-order terms with the midpoint rule then provides a fourth-order approximation to the solution of (1). Though the computations can theoretically be carried on up to any order, getting further terms soon becomes very tedious. A general procedure -which amounts to solving the Hamilton-Jacobi equation in the case where (1) is Hamiltonian- appears to be of great help.

Modified equations have also proven to be of great importance for the study of integration methods. The idea, exposed in many articles and textbooks [CMSS94, Hai94, Hai99, HLW02], is dual to the previous one. In this situation, getting the modified equation is not important per se: one is usually only interested in exhibiting some of its structural properties (such as symmetry, existence of a Hamiltonian, ...), a task accomplished without the knowledge of the coefficients themselves. However, recurrence formulas have been given by Hairer [Hai94] and by Calvo, Murua and Sanz-Serna [CMSS94] and allow to give alternative algebraic proofs of some known results. The approach followed in [Hai99] is based on a formula for the Lie-derivatives of a B-series and leads to semi-explicit formulas.

Since most numerical methods for solving the initial value problem associated with (1) may be represented using the formalism of B-series (see formula (2) for the midpoint rule), B-series play a central role in the numerical analysis of ordinary differential equations and we shall use them accordingly: a B-series $B_f(a,y)$ is a formal expression of the form

$$B_f(a,y) = a(e)y + \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau)\, F(\tau)(y) = a(e)y + ha(\bullet)f(y) + h^2 a([\bullet])f'(y)f(y) + \cdots$$

where e is the empty tree, the index set $\mathcal{T} = \{\bullet, [\bullet], [\bullet,\bullet], [[\bullet]], \cdots\}$ is the set of rooted trees , $|\cdot|$, σ and F are functions defined on $\mathcal{T}$, and where a is a function defined on $\mathcal{T} \cup \{e\}$ as well which characterizes the B-series itself. The concept of B-series was introduced in [HW74], following the pioneering work of John Butcher [But69, But72], and is now exposed in various textbooks and articles, though possibly with different normalizations (see for instance [HLW02]). A remarkable result of Calvo and Sanz-Serna [CSS94] gives an algebraic characterization of symplectic B-series, while the characterization of Hamiltonian vector fields has been obtained in [Hai94].

In this paper, we introduce a new composition law on B-series, denoted star and called *law of substitution*, obtained as the result of the substitution of a vector field $g(y) = \frac{1}{h}B_f(b,y)$ into another B-series $B_g(a,y)$. Formally, this comes to considering expressions of the form

$$\begin{aligned} B_g(a,y) &= a(e)y + a(\bullet)B_f(b,y) + a([\bullet])\partial_y(B_f(b,y))B_f(b,y) + a([\bullet,\bullet])\partial_y^2(B_f(b,y))\Big(B_f(b,y), B_f(b,y)\Big) + \ldots \\ &:= B_f(b \star a, y) \end{aligned}$$

Note that this is exactly the kind of manipulation we have considered above for the midpoint rule, where we have replaced the vector field f by $\breve{f}$ into the B-series expansion (2): denoting a the coefficients of the B-series (2), b the unknown coefficients of the modified equation (5) and $\frac{1}{\gamma}$ those of (4), this may be written as

$$B_f(b \star a, y) = B_f(\frac{1}{\gamma}, y). \tag{6}$$

Similarly, computing the vector field $\frac{1}{h}B_f(b,y)$ of the modified equation obtained by backward error analysis can also be viewed as solving the implicit equation

$$B_f(b \star \frac{1}{\gamma}, y) = B_f(a,y). \tag{7}$$

The aim of this paper is to study the newly introduced law: we give an explicit formula for the computation of $b \star a$ and study the algebraic properties of $\star$. Special attention is paid to the cases where f is a Hamiltonian vector field. We show that equation (7) can be solved explicitly and b computed in terms of a through the formula

$$B_f(b,y) = B_f((a - a(e)\delta_e) \star \omega, y) \tag{8}$$

where $B_f(a - a(e)\delta_e, y)$ is simply $B_f(a,y) - a(e)y$ and where $B_f(\omega, y)$ is the B-series of the modified equation for backward error analysis corresponding to the Euler explicit method. This corresponds to the *formal* logarithm of $B(a,y)$ as defined in [Mur03].

2 Preliminaries

In this section, we briefly recall a few definitions and properties related to trees and B-Series. A complete presentation may be found in Chapter III of [HLW02].

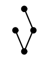
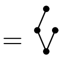
2.1 Trees and B-Series

Let e denote the empty tree.

Definition 2.1 ***(Unordered trees).*** *The set $\mathcal{T}$ of (rooted) unordered trees is recursively defined by*

$$\bullet \in \mathcal{T}, \qquad [\tau_1, \ldots, \tau_m] \in \mathcal{T} \quad \textit{for all } \tau_1, \ldots, \tau_m \in \mathcal{T}, \tag{9}$$

where $\bullet$ is the tree with only one vertex, and $\tau = [\tau_1, \ldots, \tau_m]$ represents the rooted tree obtained by grafting the roots of $\tau_1, \ldots, \tau_m \in \mathcal{T}$ to a new vertex. Trees τ_i are called the branches of τ.

We note that τ does not depend on the ordering of $\tau_1, \ldots, \tau_m$. For instance, trees $[\bullet, [\bullet]] =$  and $[[\bullet], \bullet] =$  are equal in $\mathcal{T}$.

Definition 2.2 *The following coefficients are defined recursively for all trees $\tau = [\tau_1^{\mu_1} \ldots, \tau_n^{\mu_n}] \in \mathcal{T}$, where each μ_i denotes the multiplicity of τ_i, and $m = \sum_{i=1}^n \mu_i$ denotes the exact number of branches of τ:*

$$|\tau| = 1 + \sum_{i=1}^n \mu_i |\tau_i| \qquad \textit{(the order, i.e. the number of vertices)}, \tag{10}$$

$$\sigma(\tau) = \prod_{i=1}^n \mu_i! \sigma(\tau_i)^{\mu_i} \qquad \textit{(symmetry)}, \tag{11}$$

$$\gamma(\tau) = |\tau| \prod_{i=1}^n \gamma(\tau_i)^{\mu_i} \qquad \textit{(density)}, \tag{12}$$

$$\beta(\tau) = \frac{m!}{\mu_1! \cdots \mu_n!}, \tag{13}$$

$$\nu(\tau) = \beta(\tau) \prod_{i=1}^n \nu(\tau_i)^{\mu_i}. \tag{14}$$

Initial values for $\bullet$ and a few examples are given in Table 1.

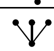
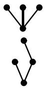
$\lvert\tau\rvert$	τ	graph	$F(\tau)(y)$	$\gamma(\tau)$	$\sigma(\tau)$	$\beta(\tau)$	$\nu(\tau)$
1	$\bullet$	$\bullet$	f	1	1	1	1
2	$[\bullet]$		$f'f$	2	1	1	1
3	$[\bullet, \bullet]$		$f''(f,f)$	3	2	1	1
3	$[[\bullet]]$		$f'f'f$	6	1	1	1
4	$[\bullet, \bullet, \bullet]$		$f'''(f,f,f)$	4	6	1	1
4	$[\bullet, [\bullet]]$		$f''(f, f'f)$	8	1	2	2
4	$[[\bullet, \bullet]]$		$f'f''(f,f)$	12	2	1	1
4	$[[[\bullet]]]$		$f'f'f'f$	24	1	1	1

Table 1: Trees of order ≤ 4, elementary differentials, and coefficients

Definition 2.3 ***(Elementary differentials).*** *For a vector field $f : \mathbb{R}^d \to \mathbb{R}^d$, and for an unordered tree $\tau = [\tau_1, \ldots, \tau_m] \in \mathcal{T}$, the so-called elementary differential is a mapping $F_f(\tau) : \mathbb{R}^d \to \mathbb{R}^d$, recursively defined by*

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

Definition 2.4 ***(B-Series, [HW74]).*** *For a mapping $a : \mathcal{T} \cup \{e\} \to \mathbb{R}$, a formal series of the form*

$$B_f(a, y) = a(e)y + \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau) F_f(\tau)(y) \tag{15}$$

is called a B-series.

Definition 2.5 *For all $u \in \mathcal{T} \cup \{e\}$, we define the mapping $\delta_u : \mathcal{T} \cup \{e\} \to \mathbb{R}$ by*

$$\begin{array}{rcl} \delta_u : \mathcal{T} \cup \{e\} & \longrightarrow & \mathbb{R} \\ \tau & \longmapsto & \begin{cases} 1 \text{ if } \tau = u, \\ 0 \text{ if } \tau \neq u. \end{cases} \end{array} \tag{16}$$

Then, for all $u \in \mathcal{T}$, it holds

$$B_f(\delta_u, y) = \frac{h^{|u|}}{\sigma(u)} F_f(u)(y). \tag{17}$$

Theorem 2.6 ***(Exact solution).*** *(see [HLW02], Theorem II.1.3, p.49)*
If $y(t)$ denotes the exact solution of (1), it holds for all $j \geq 1$,

$$\frac{1}{j!} y^{(j)}(0) = \sum_{\tau \in \mathcal{T}, |\tau| = j} \frac{1}{\sigma(\tau)\gamma(\tau)} F_f(\tau)(y_0). \tag{18}$$

Therefore, the exact solution of (1) is (formally) given by

$$y(h) = B(\frac{1}{\gamma}, y_0). \tag{19}$$

2.2 Basic tools for trees

2.2.1 Tree products

Definition 2.7 ***(Butcher 1972, Murua & Sanz-Serna 1999)*** *(see, [HLW02], Definition III.3.7, p.71)*
For $u, v \in \mathcal{T}$, with $u = [u_1, \ldots, u_k]$ and $v = [v_1, \ldots, v_l]$, we denote

$$u \circ v = [u_1, \ldots, u_k, v], \qquad \textit{(Butcher product)}, \tag{20}$$

$$u \times v = [u_1, \ldots, u_k, v_1, \ldots, v_l], \qquad \textit{(merging product)}. \tag{21}$$

Remark The merging product is both associative and commutative, whereas the Butcher product is none of the two. To simplify the notation, we write products of several factors without parentheses, when we mean evaluation form left to right:

$$\begin{array}{rcl} u \circ v_1 \circ v_2 \circ v_3 \circ \ldots \circ v_s & = & (((u \circ v_1) \circ v_2) \circ \ldots) \circ v_s, \\ u_1 \circ u_2 \times u_3 \circ u_4 & = & ((u_1 \circ u_2) \times u_3) \circ u_4, \\ & \ldots & \end{array} \tag{22}$$

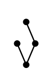
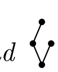
Here, factors $v_1, \ldots, v_s$ in (22) can be freely permuted.

2.2.2 Ordered trees

In order to manipulate trees more conveniently, it is useful to consider the set $\mathcal{OT}$ of ordered trees defined below (see [HLW02], III.1, p.56).

Definition 2.8 ***(Ordered trees).*** *The set $\mathcal{OT}$ of ordered trees is recursively defined by*

$$\bullet \in \mathcal{OT}, \qquad (\omega_1, \ldots, \omega_m) \in \mathcal{T} \quad \textit{for all } \omega_1, \ldots, \omega_m \in \mathcal{OT}, \tag{23}$$

In contrast to $\mathcal{T}$, the ordered tree ω depends on the ordering $\omega_1, \ldots, \omega_m$, e.g. trees  *and*  *are different in $\mathcal{OT}$.*

Neglecting the ordering, a tree $\tau \in \mathcal{T}$ can be considered as an equivalent class of ordered trees, denoted $\tau = \overline{\omega}$. Therefore, any function ψ defined on $\mathcal{T}$ (such as order, symmetry, density, ...) can be extended to $\mathcal{OT}$ by putting $\psi(\omega) = \psi(\overline{\omega})$ for all $\omega \in \mathcal{OT}$. Moreover, for all $\tau \in \mathcal{T}$, we can choose a tree $\omega(\tau) \in \mathcal{OT}$ such as $\tau = \overline{\omega(\tau)}$.

Proposition 2.9 *For all $\tau \in \mathcal{T}$, coefficient $\nu(\tau)$ represents the number of ordered trees $\omega \in \mathcal{OT}$ such that $\overline{\omega} = \tau$. Therefore, given a real function ψ on trees,*

$$\sum_{\tau \in \mathcal{T}} \psi(\tau) = \sum_{\omega \in \mathcal{OT}} \frac{1}{\nu(\omega)} \psi(\omega). \tag{24}$$

The following proposition is very similar.

Proposition 2.10 *For $\tau \in \mathcal{T}$, $\beta(\tau)$ represents the number of ordered tuples $(t_1, \ldots, t_m)$ of unordered trees $t_i \in \mathcal{T}$, such that $\tau = [t_1, \ldots, t_m]$. Therefore, given a real function ψ defined on trees,*

$$\sum_{\tau \in \mathcal{T}} \psi(\tau) = \sum_{t_1, \ldots, t_m \in \mathcal{T}} \frac{1}{\beta([t_1, \ldots, t_m])} \psi([t_1, \ldots, t_m]). \tag{25}$$

Remark Of course, (24) and (25) hold true provided there is a finite number of non-zero terms involved.

2.2.3 Partitions and skeletons

Definition 2.11 *(**Partitions of a tree**) A partition p^θ of an ordered tree $\theta \in \mathcal{OT}$ is the (ordered) tree obtained from θ by replacing some of its edges by dashed ones. We denote $P(p^\theta) = \{s_1, \ldots, s_k\}$ the list of subtrees $s_i \in \mathcal{T}$ obtained from p^θ by removing dashed edges and by neglecting the ordering of each subtree. We denote $\#(p^\theta) = k$ the number of s_i's. We observe that precisely one of the s_i's contains the root of θ. We denote this distinguished tree by $R(p^\theta) \in \mathcal{T}$. We denote $P^*(p^\theta) = P(p^\theta) \backslash \{R(p^\theta)\}$ the list of s_i's that do not contain the root of θ. Eventually, the set of all partitions p^θ of θ is denoted $\mathcal{P}(\theta)$. Finally, for $\tau \in \mathcal{T}$, we put $\mathcal{P}(\tau) = \mathcal{P}(\omega(\tau))$ where $\omega(\tau) \in \mathcal{OT}$ is given in definition 2.8.*

We observe that any tree $\tau \in \mathcal{T}$ has exactly $2^{|\tau|-1}$ partitions $p^\tau \in \mathcal{P}(\tau)$, and that different partitions may lead to the same list of subtrees $P(p^\tau)$.

Remark The partitions p^τ defined above are slightly different from those defined in [Hai94]. The list $P(p^\tau)$ is often called a *forest* in the literature [Mur03] or a *monomial in trees* obtained by a *full* cut, as defined in [CK98].

Definition 2.12 *(**Skeleton of a partition, Chartier & Lapôtre**, see [CL98], definition 12, p. 10)*
The skeleton *$\chi(p^\tau) \in \mathcal{T}$ of a partition $p^\tau \in \mathcal{P}(\tau)$ of a tree $\tau \in \mathcal{T}$ is the tree obtained by replacing in p^τ each tree of $P(p^\tau)$ by a single vertex and then dashed edges by solid ones. We can notice that $|\chi(p^\tau)| = \#(p^\tau)$.*

Definition 2.13 *(**Admissible partitions**) A partition $p^\tau \in \mathcal{P}(\tau)$ of a tree $\tau \in \mathcal{T}$ is called admissible if $\chi(p^\tau)$ is a tree of the form $\bullet, [\bullet], [\bullet,\bullet], [\bullet,\bullet,\bullet], [\bullet,\bullet,\bullet,\bullet], \ldots$ It means that any path from the root of p^τ to any vertex of p^τ has at most one dashed edge. The set of admissible partitions p^τ of τ is denoted $\mathcal{AP}(\tau)$.*

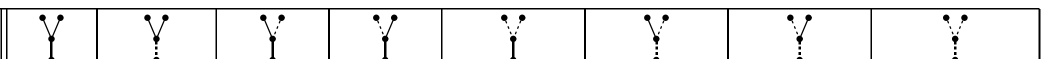
$p^\tau \in \mathcal{P}(\tau)$								
$\#(p^\tau)$	1	2	2	2	3	3	3	4
$\chi(p^\tau)$	$\bullet$	$[\bullet]$	$[\bullet]$	$[\bullet]$	$[\bullet,\bullet]$	$[[\bullet]]$	$[[\bullet]]$	$[[\bullet,\bullet]]$
$R(p^\tau)$	$[[\bullet,\bullet]]$	$\bullet$	$[[\bullet]]$	$[[\bullet]]$	$[\bullet]$	$\bullet$	$\bullet$	$\bullet$
$P(p^\tau)$	$\{[[\bullet,\bullet]]\}$	$\{\bullet, [\bullet,\bullet]\}$	$\{\bullet, [[\bullet]]\}$	$\{\bullet, [[\bullet]]\}$	$\{\bullet, \bullet, [\bullet]\}$	$\{\bullet, \bullet, [\bullet]\}$	$\{\bullet, \bullet, [\bullet]\}$	$\{\bullet, \bullet, \bullet, \bullet\}$
$P^*(p^\tau)$	$\emptyset$	$\{[\bullet,\bullet]\}$	$\{\bullet\}$	$\{\bullet\}$	$\{\bullet, \bullet\}$	$\{\bullet, [\bullet]\}$	$\{\bullet, [\bullet]\}$	$\{\bullet, \bullet, \bullet\}$

Table 2: The 8 partitions of tree $\tau = [[\bullet, \bullet]]$ with corresponding skeletons and lists

2.3 The Butcher Group

Theorem 2.14 *(**Composition of B-Series [HW74]**, see [HLW02], Theorem III.1.10, p.58).*
Let $a, b : \mathcal{T} \cup \{e\} \to \mathbb{R}$ be two mappings, with $a(e) = 1$. Then the B-series $B(a, y)$ inserted into $B(b, \cdot)$ is again a B-series

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

and $a \cdot b : \mathcal{T} \cup \{e\} \to \mathbb{R}$ is defined by

$$a \cdot b(e) = b(e), \qquad \forall \tau \in \mathcal{T},\ a \cdot b(\tau) = b(e)a(\tau) + \sum_{p^\tau \in \mathcal{AP}(\tau)} b(R(p^\tau)) \prod_{\delta \in P^*(p^\tau)} a(\delta). \tag{26}$$

Theorem 2.15 ***(inverse for Composition law (26)****, see [CK98]). Let $a : \mathcal{T} \cup \{e\} \to \mathbb{R}$ be a mapping with $a(e) = 1$. Then, a is invertible for composition law (26), and the inverse element is given by*

$$a^{-1}(e) = 1, \qquad \forall \tau \in \mathcal{T},\ a^{-1}(\tau) = \sum_{p^\tau \,\in\, \mathcal{P}(\tau)} (-1)^{\#(p^\tau)} \prod_{\delta \in P(p^\tau)} a(\delta). \tag{27}$$

Composition law (26) on B-series can therefore be turned into a group operation.

Theorem 2.16 ***(Butcher Group)*** *The set of mappings $a : \mathcal{T} \cup \{e\} \to \mathbb{R}$, satisfying $a(e) = 1$, is a group for composition law (26). Its unit element is δ_e, defined in (16).*

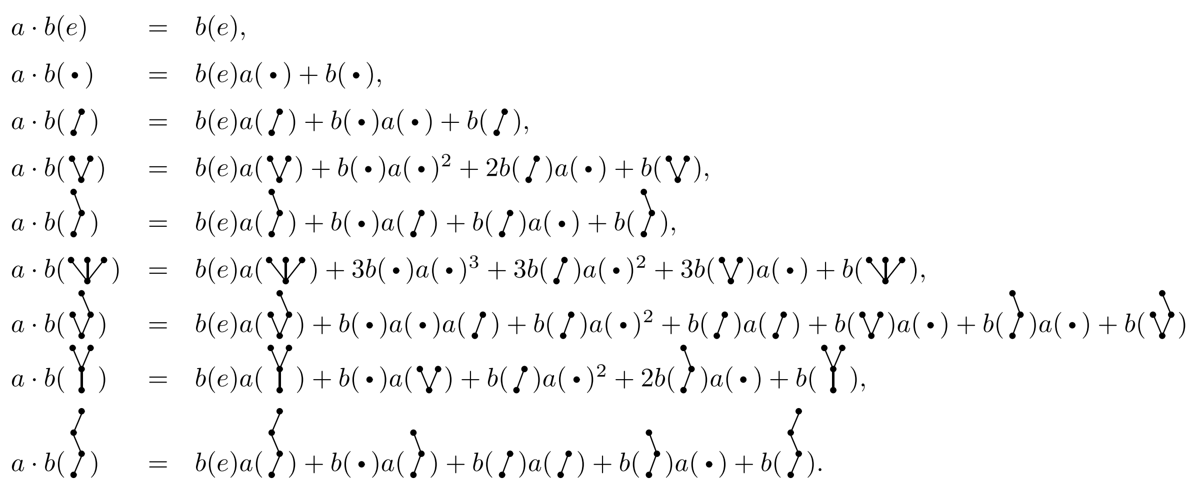


Table 3: Composition law (26) for trees of order ≤ 4.

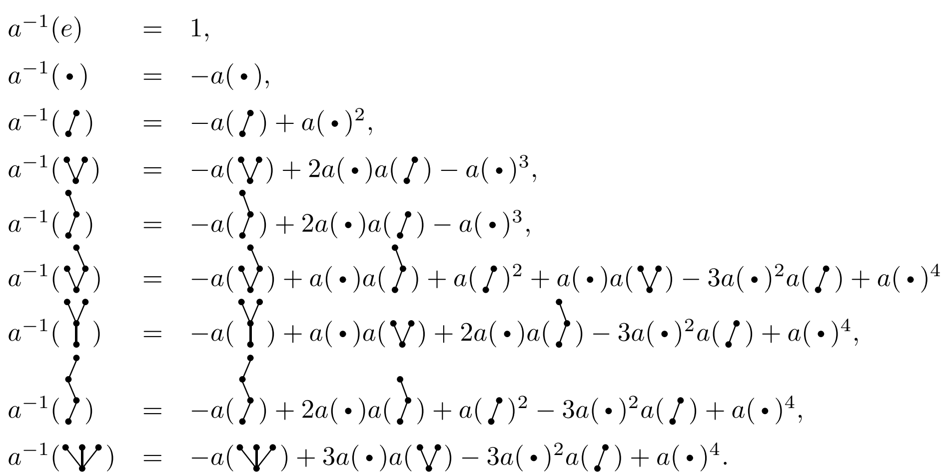


Table 4: Inverse (27) for composition law (26) for trees of order ≤ 4.

3 A substitution law for modified fields

3.1 Main result

Theorem 3.1 ***(Substitution law)****.*

$$
\begin{aligned}
b\star a(e) &= a(e),\\
b\star a(\bullet) &= a(\bullet)b(\bullet),\\
b\star a([\bullet]) &= a(\bullet)b([\bullet]) + a([\bullet])b(\bullet)^2,\\
b\star a([\bullet\bullet]) &= a(\bullet)b([\bullet\bullet]) + 2a([\bullet])b(\bullet)b([\bullet]) + a([\bullet\bullet])b(\bullet)^3,\\
b\star a([[\bullet]]) &= a(\bullet)b([[\bullet]]) + 2a([\bullet])b(\bullet)b([\bullet]) + a([[\bullet]])b(\bullet)^3,\\
b\star a([[\bullet]\bullet]) &= a(\bullet)b([[\bullet]\bullet]) + a([\bullet])b(\bullet)b([[\bullet]]) + a([\bullet])b([\bullet])^2 + a([\bullet])b(\bullet)b([\bullet\bullet]) + 2a([\bullet\bullet])b(\bullet)^2b([\bullet])\\
&\quad + a([[\bullet]])b(\bullet)^2b([\bullet]) + a([[\bullet]\bullet])b(\bullet)^4,\\
b\star a([[\bullet\bullet]]) &= a(\bullet)b([[\bullet\bullet]]) + a([\bullet])b(\bullet)b([\bullet\bullet]) + 2a([\bullet])b(\bullet)b([[\bullet]]) + a([\bullet\bullet])b(\bullet)^2b([\bullet])\\
&\quad + 2a([[\bullet]])b(\bullet)^2b([\bullet]) + a([[\bullet\bullet]])b(\bullet)^4,\\
b\star a([[[\bullet]]]) &= a(\bullet)b([[[\bullet]]]) + 2a([\bullet])b(\bullet)b([[\bullet]]) + a([\bullet])b([\bullet])^2 + 3a([[\bullet]])b(\bullet)^2b([\bullet]) + a([[[\bullet]]])b(\bullet)^4,\\
b\star a([\bullet\bullet\bullet]) &= a(\bullet)b([\bullet\bullet\bullet]) + 3a([\bullet])b(\bullet)b([\bullet\bullet]) + 3a([\bullet\bullet])b(\bullet)^2b([\bullet]) + a([\bullet\bullet\bullet])b(\bullet)^4.
\end{aligned}
$$

Table 5: Substitution law $\star$ defined in (28) for trees of order ≤ 4.

Let $a, b : \mathcal{T}\cup\{e\} \to \mathbb{R}$ be two mappings with $b(e) = 0$. Given a field $f : \mathbb{R}^d \to \mathbb{R}^d$, consider the (h-dependent) field $g : \mathbb{R}^d \to \mathbb{R}^d$ defined by

$$hg(y) = B_f(b, y).$$

Then, there exists a mapping $b\star a : \mathcal{T}\cup\{e\} \to \mathbb{R}$ satisfying

$$B_g(a, y) = B_f(b\star a, y),$$

and $b\star a$ is defined by

$$b\star a(e) = a(e), \qquad \forall\tau\in\mathcal{T},\ b\star a(\tau) = \sum_{p^\tau\,\in\mathcal{P}(\tau)} a(\chi(p^\tau)) \prod_{\delta\in P(p^\tau)} b(\delta). \tag{28}$$

Remark We notice a resemblance between formula (28) and formula (27) giving the inverse in the Butcher group. This is discussed further, in the remark that follows Proposition 3.5.

To illustrate Theorem 3.1, we now compute by hand the coefficients obtained by the substitution law, for trees up to order 3. We have

$$B_g(a,y) = a(e)y + ha(\bullet)g(y) + h^2a([\bullet])g'(y)g(y) + \frac{h^3}{2}a([\bullet\bullet])g''(y)(g(y),g(y)) + h^3a([[\bullet]])g'(y)g'(y)g(y) + \ldots \tag{29}$$

We then compute each term individually. For brevity we suppress the argument (y).

$$
\begin{aligned}
hg &= hb(\bullet)f + h^2b([\bullet])f'f + \frac{h^3}{2}b([\bullet\bullet])f''(f,f) + h^3b([[\bullet]])f'f'f + \ldots\\
h^2g'g &= h^2(b(\bullet)f + hb([\bullet])f'f + ...)'(b(\bullet)f + hb([\bullet])f'f + \ldots)\\
&= h^2b(\bullet)f'b(\bullet)f + h^2b(\bullet)f'hb([\bullet])f'f + h^3b([\bullet])(f'f)'b(\bullet)f + \ldots\\
&= h^2b(\bullet)^2f'f + 2h^3b(\bullet)b([\bullet])f'f'f + h^3b([\bullet])b(\bullet)f''(f',f) + \ldots\\
\frac{h^3}{2}g''(g,g) &= \frac{h^3}{2}(b(\bullet)f + \ldots)''(b(\bullet)f + \ldots, b(\bullet)f + \ldots) = \frac{h^3}{2}b(\bullet)^3f''(f,f) + \ldots\\
h^3g'g'g &= h^3(b(\bullet)f + \ldots)'(b(\bullet)f + \ldots)'(b(\bullet)f + \ldots) = h^3b(\bullet)^3f'f'f + \ldots
\end{aligned} \tag{30}
$$

We then substitute expressions of hg, $h^2g'g$, $h^3g'g'g$, $\frac{h^3}{2}g''(g,g)$ into (29), and collect terms in hf, $h^2f'f$, $h^3f'f'f$, $\frac{h^3}{2}f''(f,f)$. This gives

$$B_g(a,y) \;=\; a(e) + ha(\bullet)b(\bullet)f + h^2\Big(a(\bullet)b([\bullet]) + a([\bullet])b(\bullet)^2\Big)f'f$$

$$+\frac{h^3}{2}\Big(a(\bullet)b([\bullet,\bullet]) + 2a([\bullet])b(\bullet)b([\bullet]) + a([\bullet,\bullet])b(\bullet)^3\Big)f''(f',f') \qquad (31)$$
$$+h^3\Big(a(\bullet)b([[\bullet]]) + 2a([\bullet])b(\bullet)b([\bullet]) + a([[\bullet]])b(\bullet)^3\Big)f'f'f + \dots$$

We recognize formulas appearing in Table 5.

We may now prove Theorem 3.1. We begin with the following lemma, that uses the notion of admissible partitions $p^v \in \mathcal{AP}(v)$ of a tree $v \in \mathcal{T}$, as defined in section 2.2.3.

Lemma 3.2 ***(Derivative of a B-series in the direction of a tree)***
Let $t = [t_1, \dots, t_m] \in \mathcal{T}$ be a tree with exactly $m \geq 0$ branches. Consider the field $g(y)$ defined in Theorem 3.1, i.e. $hg(y) = B_f(b, y)$. Then, there exists $d_t b : \mathcal{T} \cup \{e\} \to \mathbb{R}$ satisfying

$$\frac{h^{|t|}}{\sigma(t)}\, g^{(m)}(y)\ (F_f(t_1)(y), \dots, F_f(t_m)(y)) = B_f(d_t b, y), \qquad (32)$$

and $d_t b$ is defined by

$$d_t b(e) = 0, \qquad \forall v \in \mathcal{T},\ d_t b(v) = \sum_{\substack{p^v \in \mathcal{AP}(v),\\ P^*(p^v) = \{t_1,\dots,t_m\}}} b(R(p^v)), \qquad (33)$$

where the sum is over all admissible partitions $p^v \in \mathcal{AP}(v)$ of v such that the list of trees $P^*(p^v)$ is exactly the list of branches $\{t_1, \dots, t_m\}$ of t.

values of $d_t b(v)$	$t = \bullet$	$t = [\bullet]$	$t = [\bullet,\bullet]$	$t = [[\bullet]]$
$v = e$	0	0	0	0
$v = \bullet$	$b(\bullet)$	0	0	0
$v = [\bullet]$	$b([\bullet])$	$b(\bullet)$	0	0
$v = [\bullet,\bullet]$	$b([\bullet,\bullet])$	$2b([\bullet])$	$b(\bullet)$	0
$v = [[\bullet]]$	$b([[\bullet]])$	$b([\bullet])$	0	$b(\bullet)$
$v = [\bullet,\bullet,\bullet]$	$b([\bullet,\bullet,\bullet])$	$3b([\bullet,\bullet])$	$3b([\bullet])$	0
$v = [\bullet,[\bullet]]$	$b([\bullet,[\bullet]])$	$b([\bullet,\bullet]) + b([[\bullet]])$	$b([\bullet])$	$b([\bullet])$
$v = [[\bullet,\bullet]]$	$b([[\bullet,\bullet]])$	$2b([[\bullet]])$	$b([\bullet])$	0
$v = [[[\bullet]]]$	$b([[[\bullet]]])$	$b([[\bullet]])$	0	$b([\bullet])$
$v = [\bullet,\bullet,[\bullet]]$	$b([\bullet,\bullet,[\bullet]])$	$b([\bullet,\bullet,\bullet]) + 2b([\bullet,[\bullet]])$	$2b([\bullet,\bullet]) + b([[\bullet]])$	$b([\bullet,\bullet])$
$v = [[\bullet,\bullet,\bullet]]$	$b([[\bullet,\bullet,\bullet]])$	$3b([[\bullet,\bullet]])$	$3b([[\bullet]])$	0
$v = [\bullet,[[\bullet]]]$	$b([\bullet,[[\bullet]]])$	$b([\bullet,[\bullet]]) + b([[[\bullet]]])$	$b([[\bullet]])$	$b([\bullet,\bullet])$

Table 6: Examples for formula (33) in lemma 3.2.

Remark We may comment on the following special cases:

- $b = \delta_\bullet$: $d_t\delta_\bullet = \delta_t$.
- $m = 0$, $t = \bullet$: $d_\bullet b = b$.
- The case $m = 1$ corresponds to a Lie-Derivative of a B-series, defined for instance in Lemma IX.9.1, p. 315 of [HLW02], and for all $t = [t_1] \in \mathcal{T}$ we have $d_t b = \partial_{\delta_{t_1}} b$.

Proof of Lemma 3.2

We adapt the proof of lemma IX.9.1 of [HLW02]. Let Q be the left member of (32):

$$Q = \frac{h^{|t|}}{\sigma(t)}\ g^{(m)}(y)\ (F_f(t_1)(y), \dots, F_f(t_m)(y)).$$

Using Leibniz' rule together with Proposition 2.9 gives

$$Q = \sum_{\theta \in \mathcal{OT}} \frac{h^{|\theta|+|t|-1} b(\theta)}{\nu(\theta)\sigma(\theta)} \sum_{\gamma_1,\dots,\gamma_m} \sum_{\substack{\delta \in \mathcal{OT}, \\ \overline{\delta} = t}} \frac{1}{\nu(\delta)\sigma(\delta)} F_f(\theta \circ^1_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m))(y),$$

were $\delta = (\delta_1, \dots, \delta_m)$, and the sum $\sum_{\gamma_1,\dots,\gamma_m}$ is over all m-tuples $(\gamma_1, \dots, \gamma_m)$ of vertices of θ. Expression $\theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m)$ denotes the ordered tree obtained when attaching the m roots of the δ_i's respectively to the m vertices γ_i with m new branches. This operation can be done in $\eta(\gamma_1, \dots, \gamma_m)$ different ways, depending on the number of upwards leaving branches on each vertex γ_i. The exponent k means we choose the k^{th} way to do this. Hence, by putting $\kappa(u) = \nu(u)\sigma(u)$ for all $u \in \mathcal{T}$, we get

$$Q = \sum_{\theta \in \mathcal{OT}} \frac{h^{|\theta|+|t|-1} b(\theta)}{\kappa(\theta)} \sum_{\gamma_1,\dots,\gamma_m} \sum_{\substack{\delta \in \mathcal{OT}, \\ \overline{\delta} = t}} \frac{1}{\kappa(\delta)} F_f(\theta \circ^1_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m))(y).$$

We now attach trees δ_i on θ in all $\eta(\gamma_1, \dots, \gamma_m)$ possible ways. This gives

$$Q = \sum_{\theta \in \mathcal{OT}} h^{|\theta|+|t|-1} \sum_{\gamma_1,\dots,\gamma_m} \sum_{\substack{\delta \in \mathcal{OT}, \\ \overline{\delta} = t}} \sum_{k=1}^{\eta(\gamma_1,\dots,\gamma_m)} \frac{b(\theta)}{\kappa(\theta)\kappa(\delta)\eta(\gamma_1, \dots, \gamma_m)} F_f(\theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m))(y),$$

Then, collecting terms with equal ordered trees $\omega = \theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m)$ leads to

$$Q = \sum_{\omega \in \mathcal{OT}} h^{|\omega|} \sum_{\substack{\exists k,\ \theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m) = \omega \\ \overline{\delta} = t}} \frac{b(\theta)}{\kappa(\theta)\kappa(\delta)\eta(\gamma_1, \dots, \gamma_m)} F_f(\omega)(y),$$

where $\delta = (\delta_1, \dots, \delta_m)$ and $\sum_{\exists k,\ \theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1,\dots,\delta_m) = w,\ \overline{\delta} = t}$ is over all triplets $(\theta,\ (\gamma_1, \dots, \gamma_m),\ (\delta_1, \dots, \delta_m))$ such that there exists a way k to attach trees δ_i such that

$$\theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m) = w \quad \text{and} \quad \overline{\delta} = t.$$

Since $\kappa(u) = n!\kappa(u_1) \cdots \kappa(u_n)$ for all tree $u = [u_1, \dots, u_n] \in \mathcal{T}$, we obtain

$$\kappa(\omega) = \kappa(\theta)\kappa(\delta_1) \cdots \kappa(\delta_m)\eta(\gamma_1, \dots, \gamma_m), \qquad \text{where } \omega = \theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m). \tag{34}$$

Hence,

$$Q = \sum_{\omega \in \mathcal{OT}} \frac{h^{|\omega|}}{\kappa(\omega)} \sum_{\substack{\exists k,\ \theta \circ^k_{(\gamma_1,\dots,\gamma_m)} (\delta_1, \dots, \delta_m) = \omega \\ \overline{\delta} = t}} \frac{b(\theta)}{m!} F_f(\omega)(y).$$

Finally, because there are $m!$ possible permutations of the set of indices $\{1, \dots, m\}$, we obtain

$$\begin{aligned} Q &= \sum_{w \in \mathcal{OT}} \frac{h^{|w|}}{\kappa(w)} \sum_{\substack{p^w \in \mathcal{AP}(w), \\ P^*(p^w) = \{t_1, \dots, t_m\}}} b(R(p^w))\, F_f(w)(y) \\ &= \sum_{v \in \mathcal{T}} \frac{h^{|v|}}{\sigma(v)} \sum_{\substack{p^v \in \mathcal{AP}(v), \\ P^*(p^v) = \{t_1, \dots, t_m\}}} b(R(p^v))\, F_f(v)(y), \end{aligned}$$

which gives the result. □

Proof of Theorem 3.1

By induction on $|u|$, we prove that for all $u \in \mathcal{T}$ there exists a mapping $b \star \delta_u : \mathcal{T} \cup \{e\} \to \mathbb{R}$ satisfying

$$\frac{h^{|u|}}{\sigma(u)} F_g(u)(y) = B_f(b \star \delta_u, y), \tag{35}$$

with $b \star \delta_u$ defined by

$$b \star \delta_u(e) = 0, \qquad \forall v \in \mathcal{T},\ b \star \delta_u(v) = \sum_{\substack{p^v \in \mathcal{P}(v) \\ \chi(p^v) = u}} \prod_{\delta \in P(p^v)} b(\delta). \tag{36}$$

For $u = \bullet$, we have $hF_g(\bullet)(y) = hg(y) = B_f(b, y)$, and therefore, $b \star \delta_\bullet = b$.

We now consider a tree $u = [u_1, \ldots, u_m] \in \mathcal{T} \backslash \{\bullet\}$, and assume the result is true for trees of order $< |u|$. By definition,

$$\frac{h^{|u|}}{\sigma(u)} F_g(u)(y) = \frac{h^{|u|}}{\sigma(u)} g^{(m)}(y)(F_g(u_1)(y), \ldots, F_g(u_m)(y)).$$

Using the induction hypothesis

$$\frac{h^{|u_i|}}{\sigma(u_i)} F_g(u_i)(y) = \sum_{t_i \in \mathcal{T}} \frac{h^{|t_i|}}{\sigma(t_i)} (b \star \delta_{u_i})(t_i) F_f(t_i)(y),$$

we get, by m-linearity of $g^{(m)}(y)$,

$$\begin{aligned} \frac{h^{|u|}}{\sigma(u)} F_g(u)(y) &= \frac{\sigma(u_1) \cdots \sigma(u_m)}{\sigma(u)} \sum_{t_1, \ldots, t_m \in \mathcal{T}} \frac{1}{\sigma(t_1) \cdots \sigma(t_m)} \left(\prod_{i=1}^m (b \star \delta_{u_i})(t_i) \right) \\ & \qquad h^{|t|} g^{(m)}(y)(F_f(t_1)(y), \ldots, F_f(t_m)(y)) \end{aligned}$$

with $t = [t_1, \ldots, t_m]$. Lemma 3.2 then shows that there exists a mapping $b \star \delta_u : \mathcal{T} \cup \{e\} \to \mathbb{R}$ satisfying (35). We now prove that $b \star \delta_u$ satisfies (36). For $v \in \mathcal{T}$,

$$b \star \delta_u(v) = \frac{\sigma(u_1) \cdots \sigma(u_m)}{\sigma(u)} \sum_{t_1, \ldots, t_m \in \mathcal{T}} \frac{\sigma(t)}{\sigma(t_1) \cdots \sigma(t_m)} \left(\prod_{i=1}^m (b \star \delta_{u_i})(t_i) \right) d_t b(v),$$

with $t = [t_1, \ldots, t_m]$. Using Proposition 2.10 twice, we get

$$\begin{aligned} b \star \delta_u(v) &= \beta(u) \sum_{t_1, \ldots, t_m \in \mathcal{T}} \frac{1}{\beta(t)} \left(\prod_{i=1}^m (b \star \delta_{u_i})(t_i) \right) d_t b(v) \\ &= \beta(u) \sum_{t = [t_1, \ldots, t_m] \in \mathcal{T}} \left(\prod_{i=1}^m (b \star \delta_{u_i})(t_i) \right) d_t b(v), \\ &= \sum_{t = [t_1, \ldots, t_m] \in \mathcal{T}} \sum_{\substack{s_1, \ldots, s_m \in \mathcal{T}, \\ [s_1, \ldots, s_m] = u}} \left(\prod_{i=1}^m (b \star \delta_{s_i})(t_i) \right) d_t b(v). \end{aligned}$$

Hence, using (33),

$$b \star \delta_u(v) = \sum_{t = [t_1, \ldots, t_m] \in \mathcal{T}} \sum_{\substack{p^v \in \mathcal{AP}(v), \\ P^*(p^v) = \{t_1, \ldots, t_m\}}} \sum_{\substack{s_1, \ldots, s_m \in \mathcal{T}, \\ [s_1, \ldots, s_m] = u}} b(R(p^v)) \prod_{i=1}^m (b \star \delta_{s_i})(t_i).$$

Using once again the induction hypothesis, we finally get

$$\begin{aligned} b\star\delta_u(v) &= \sum_{\substack{t=[t_1,\dots,t_m]\in\mathcal{T},\\ p^v\in\mathcal{AP}(v),\\ P^*(p^v)=\{t_1,\dots,t_m\}}} \sum_{\substack{s_1,\dots,s_m\in\mathcal{T},\\ [s_1,\dots,s_m]=u}} \sum_{\substack{p^{t_1}\in\mathcal{P}(t_1),\ \dots,\ p^{t_m}\in\mathcal{P}(t_m),\\ \chi(p^{t_1})=s_1,\ \dots,\ \chi(p^{t_m})=s_m}} b(R(p^v))\prod_{i=1}^m \prod_{\delta\in P(p^{t_i})} b(\delta) \\ &= \sum_{\substack{t=[t_1,\dots,t_m]\in\mathcal{T},\\ p^v\in\mathcal{AP}(v),\\ P^*(p^v)=\{t_1,\dots,t_m\}}} \sum_{\substack{p^{t_1}\in\mathcal{P}(t_1),\ \dots,\ p^{t_m}\in\mathcal{P}(t_m),\\ [\chi(p^{t_1}),\dots,\chi(p^{t_m})]=u}} b(R(p^v))\prod_{i=1}^m \prod_{\delta\in P(p^{\tau_i})} b(\delta). \end{aligned}$$

We recognize the partitions $p^v\in\mathcal{P}(v)$ of tree v expressed in terms of partitions $p^{\delta_i}\in\mathcal{P}(\delta_i)$ of the δ_i's, where $P^*(p^v)=\{\delta_1,\dots,\delta_m\}$. This gives

$$b\star\delta_u(v)=\sum_{\substack{p^v\in\mathcal{P}(v)\\ \chi(p^v)=u}}\prod_{\delta\in P(p^v)} b(\delta),$$

and therefore $b\star\delta_u$ satisfies (36).

To complete the proof of Theorem 3.1 we recall that

$$B_g(a,y)=a(e)y+\sum_{u\in\mathcal{T}}\frac{h^{|u|}}{\sigma(u)}a(u)F_g(u)(y).$$

Relation $\frac{h^{|u|}}{\sigma(u)}F_g(u)(y)=B_g(\delta_u,y)=B_f(b\star\delta_u,y)$ then gives the result. □

3.2 Algebraic properties

Definition 3.3 *We define the set* Fields *of mappings associated to (non-degenerated) fields by*

$$\mathsf{Fields}=\{c:\mathcal{T}\cup\{e\}\to\mathbb{R},\ c(e)=0,\ c(\bullet)\neq 0\},\tag{37}$$

In this section, we shall prove that the following

Theorem 3.4 *The set* Fields *is a group for the law $\star$ defined in (28).*

We start with a few algebraic properties.

Proposition 3.5 *Let $a,b,\widetilde{b},c,\widetilde{c}:\mathcal{T}\cup\{e\}\to\mathbb{R}$ be mappings satisfying $a(e)=1$ and $b(e)=\widetilde{b}(e)=0$. The following properties hold:*

$$\begin{aligned} b\star\delta_e &= \delta_e, && (\delta_e \text{ absorbing element for } \star), && (38)\\ b\star\delta_\bullet &= b,\quad \delta_\bullet\star c=c, && (\delta_\bullet \text{ unit element for } \star), && (39)\\ b\star(\lambda c+\mu\widetilde{c}) &= \lambda(b\star c)+\mu(b\star\widetilde{c}),\quad \forall\lambda,\mu\in\mathbb{R}, && (\text{right-sided linearity of } \star), && (40)\\ (\widetilde{b}\star b)\star c &= \widetilde{b}\star(b\star c), && (\text{associativity of } \star), && (41)\\ b\star(a\cdot c) &= (b\star a)\cdot(b\star c), && (\text{right-sided distributivity of } \star \text{ on } \cdot), && (42)\\ (b\star a)^{-1} &= b\star a^{-1}, && && (43)\\ a^{-1} &= (a-\delta_e)\star(\delta_e+\delta_\bullet)^{-1}. && && (44) \end{aligned}$$

Remark We recall that the notation a^{-1} denotes the inverse (27) for the standard composition $\cdot$ of B-series defined in (26). We can notice that the last formula (44) is equivalent to formula (27) which gives the inverse a^{-1}:

$$\forall\tau\in\mathcal{T},\ a^{-1}(\tau)=\sum_{p^\tau\in\mathcal{P}(\tau)}(-1)^{\#(p^\tau)}\prod_{\delta\in P(p^\tau)}a(\delta).$$

Indeed, given a tree τ, we have $(\delta_e+\delta_\bullet)^{-1}(\tau)=(-1)^{|\tau|}$, and for all partition p^τ of τ, $|\chi(p^\tau)|=\#(p^\tau)$. Therefore, formula (44) together with (28) gives formula (27).

Proof of Proposition (3.5).
Formulas (38), (39), (40) are an immediate consequence of (28).

Proof of (41).
Consider the fields $g, \widetilde{g} : \mathbb{R}^d \to \mathbb{R}^d$ defined by

$$\begin{aligned} h\widetilde{g}(y) &= B_f(\widetilde{b}, y), \\ hg(y) &= B_{\widetilde{g}}(b, y). \end{aligned}$$

On one hand, we have $hg(y) = B_f(\widetilde{b} \star b, y)$, and therefore, $B_g(c, y) = B_f((\widetilde{b} \star b) \star c, y)$. On the other hand, we have $B_g(c, y) = B_{\widetilde{g}}(b \star c, y)$, which leads to $B_g(c, y) = B_f(\widetilde{b} \star (b \star c), y)$. □

Proof of (42).
Consider the field $g : \mathbb{R}^d \to \mathbb{R}^d$ defined by

$$hg(y) = B_f(b, y).$$

We have $B_g(a \cdot c, y) = B_g(a, B_g(c, y))$. However, for all mapping $s : \mathcal{T} \cup \{e\} \to \mathbb{R}$, $B_g(s, y) = B_f(b \star s, y)$. By taking s respectively equal to $a \cdot c$, and c, and a, we then get

$$B_f(b \star (a \cdot c), y) = B_f(b \star a, B_f(b \star c, y)).$$

Therefore, $B_f(b \star (a \cdot c), y) = B_f((b \star a) \cdot (b \star c), y)$, which leads to (42). □

Proof of (43).
The mapping a is invertible for composition law $\cdot$ because $a(e) = 1$. Applying (42) to $c = a^{-1}$ together with (38) gives the result. □

Proof of (44).
We first notice $(a - \delta_e) \star (\delta_e + \delta_\bullet) \stackrel{(40)}{=} (a - \delta_e) \star \delta_e + (a - \delta_e) \star \delta_\bullet \stackrel{(38)-(39)}{=} \delta_e + (a - \delta_e) = a$. Therefore, formula (43) gives the result. □

Finally, the following Proposition 3.6 gives Theorem 3.4.

Proposition 3.6 ***(Inverse element for substitution law*** $\star$***)***
Let $b : \mathcal{T} \cup \{e\} \to \mathbb{R}$ *be a mapping with* $b(e) = 0$*. Then* b *is invertible for* $\star$ *if and only if* $b(\bullet) \neq 0$*, i.e.* $b \in \mathsf{Fields}$.

Proof of Proposition 3.6
Condition $b(\bullet) \neq 0$ is obviously necessary, since for all $a : \mathcal{T} \cup \{e\} \to \mathbb{R}$, we have $b \star a(\bullet) = a(\bullet) b(\bullet)$. Conversaly, let $b \in \mathsf{Fields}$. For $a \in \mathsf{Fields}$, according to (28), we have:

$$\begin{aligned} \forall \tau \in \mathcal{T} \backslash \{\bullet\},\ b \star a(\tau) &= a(\tau) b(\bullet)^{|\tau|} + a(\bullet) b(\tau) \\ &\quad + \text{expression in } a(s), b(t), \text{ with } |s| < |\tau| \text{ and } |t| < |\tau|. \end{aligned} \tag{45}$$

By putting $a(\bullet) = \frac{1}{b(\bullet)}$, it is therefore possible to compute coefficients $a(\tau)$ by induction on $|\tau|$, such as $b \star a = a \star b = \delta_\bullet$. □

4 Applications of the substitution law

In this section, let $a : \mathcal{T} \cup \{e\} \to \mathbb{R}$ be a mapping satisfying $a(e) = 1$, $a(\bullet) \neq 0$, and let $f : \mathbb{R}^d \to \mathbb{R}^d$ be a field. We consider here the numerical flow Φ_h^g, where $g : \mathbb{R}^d \to \mathbb{R}^d$ denotes a field, whose B-series expansion is

$$\Phi_h^g(y) = B_g(a, y). \tag{46}$$

4.1 Backward error analysis

The fundamental idea of backward error analysis consists in interpreting the numerical solution $y_1 = \Phi_h^f$ of the initial value problem $y(0) = y_0,\ \dot{y} = f(y)$ as the exact solution of a modified differential equation $\dot{\hat{y}} = \hat{f}(\hat{y})$:

Theorem 4.1 *There exists a modified field $\hat{f}(y) = \hat{f}_1(y) + h\hat{f}_2(y) + h^2\hat{f}_3(y) + \dots$ such that*

$$\Phi_h^f(y_0) = \hat{y}(h),$$

where $\hat{y}(t)$ denotes the exact solution of

$$\left\{ \begin{array}{ccc} \dot{\hat{y}} & = & \hat{f}(\hat{y}) \\ \hat{y}(0) & = & y_0 \end{array} \right. . \tag{47}$$

Moreover, $\hat{f}(y)$ is defined by

$$h\hat{f}(y) = B_f(\hat{b}, y),$$

where $\hat{b} \in \mathsf{Fields}$ is the solution of

$$\hat{b} \star \frac{1}{\gamma} = a. \tag{48}$$

Proof of Theorem 4.1

We have

$$\Phi_h^f(y_0) = B_f(a, y),$$

and

$$\hat{y}(h) = B_{\hat{f}}(\frac{1}{\gamma}, y_0) = B_f(\hat{b} \star \frac{1}{\gamma}, y_0).$$

Therefore, Theorem 4.1 is equivalent to finding $\hat{b}$ solution of

$$\hat{b} \star \frac{1}{\gamma} = a,$$

i.e., by subtracting δ_e,

$$\hat{b} \star (\frac{1}{\gamma} - \delta_e) = (a - \delta_e).$$

Since $\frac{1}{\gamma} - \delta_e$ and $a - \delta_e$ are in the group Fields this equation possesses a solution $\hat{b}$. □

Remark Let $\omega \in \mathsf{Fields}$ denote the inverse element of $\frac{1}{\gamma} - \delta_e$ for $\star$. This gives a new formula to compute the coefficients $\hat{b}(\tau)$:

$$\hat{b} = (a - \delta_e) \star \omega. \tag{49}$$

Since, $\omega \star (\frac{1}{\gamma} - \delta_e) = \delta_\bullet$, by adding δ_e, we get

$$\omega \star \frac{1}{\gamma} = \delta_e + \delta_\bullet. \tag{50}$$

Therefore the coefficients $\omega(\tau)$ can be interpreted as the coefficients of the modified field for backward error analysis, for the Euler explicit method $y_1 = y_0 + hf(y_0)$, corresponding to $a = \delta_e + \delta_\bullet$. They may be computed by induction using Proposition 4.18. Note that the same ω already appears in [Mur03] with the same definition and a recurrence formula is also given therein.

The properties of ω are inherited from those of $\frac{1}{\gamma}$. We recall in particular the following property:

Lemma 4.2 *The coefficients $\frac{1}{\gamma}$ of the exact flow satisfy the following relation for all $m \geq 2$:*

$$\forall (t_1, \dots, t_m) \in \mathcal{T}^m, \quad \sum_{i=1}^m \frac{1}{\gamma}(t_i \circ \prod_{j \neq i} t_j) = \prod_{i=1}^m \frac{1}{\gamma}(t_i). \tag{51}$$

For the sake of brevity, we shall sometimes use in the sequel the following notation:

$$a\Big(\sum_i t_i\Big) := \sum_i a(t_i)$$

for any mapping $a : \mathcal{T} \to \mathbb{R}$ and any t_i's in $\mathcal{T}$.

Relations (51) fully determine the (scaled) γ-function. For $m = 2$, the induced relation for ω is given in the next proposition:

Proposition 4.3 *The coefficients ω of the modified field (obtained by backward analysis) of the explicit Euler method satisfy the following relation:*

$$\forall\,(u,v) \in \mathcal{T}^2, \quad \omega(u \circ v) + \omega(v \circ u) + \omega(u \times v) = 0. \tag{52}$$

Proof

Let t be a tree of the form $t = u \circ v$. The main idea of the proof is to notice that a partition p^t of t if either of the form $p^u \circ p^v$, whenever p^t embeds an dashed edge between the roots of u and v, or of the form $p^u \bullet p^v$, whenever there is a solid edge in p^t between the roots of u and v. We have the relations:

p^t	$\chi(p^t)$	$R(p^t)$	$P^*(p^t)$
$p^u \circ p^v$	$\chi(p^u) \times \chi(p^v)$	$R(p^u) \circ R(p^v)$	$P^*(p^u) \cup P^*(p^v)$
$p^u \bullet p^v$	$\chi(p^u) \circ \chi(p^v)$	$R(p^u)$	$P^*(p^u) \cup P(p^v)$

(53)

Formula (28) with $a = \omega$ and $b = \frac{1}{\gamma} - \delta_e$ and for $t = u \circ v$ may then be written as

$$\Big((\frac{1}{\gamma} - \delta_e) \star \omega\Big)(u \circ v) = \sum_{p^u \in \mathcal{P}(u),\ p^v \in \mathcal{P}(v)} \Big(\frac{\omega(\chi(p^u) \times \chi(p^v))}{\gamma(R(p^u) \circ R(p^v))} + \frac{\omega(\chi(p^u) \circ \chi(p^v))}{\gamma(R(p^u))\gamma(R(p^u))}\Big) \prod_{\delta \in P^*(p^u) \cup P^*(p^v)} \frac{1}{\gamma(\delta)}. \tag{54}$$

It then follows that $\Big((\frac{1}{\gamma} - \delta_e) \star \omega\Big)(u \circ v + v \circ u)$ has the following expression:

$$\sum_{p^u,p^v} \Big(\frac{\omega(\chi(p^u) \times \chi(p^v))}{\gamma(R(p^u) \circ R(p^v) + R(p^v) \circ R(p^u))} + \frac{\omega(\chi(p^u) \circ \chi(p^v))}{\gamma(R(p^u))\gamma(R(p^v))} + \frac{\omega(\chi(p^v) \circ \chi(p^u))}{\gamma(R(p^u))\gamma(R(p^u))}\Big) \prod_{\delta \in P^*(p^u) \cup P^*(p^v)} \frac{1}{\gamma(\delta)} \tag{55}$$

$$= \sum_{p^u,p^v} \omega\Big(\chi(p^u) \times \chi(p^v) + \chi(p^u) \circ \chi(p^v) + \chi(p^v) \circ \chi(p^u)\Big) \prod_{\delta \in P^u \cup P^v} \frac{1}{\gamma(\delta)},$$

where we have used relation (51) with u and v. Now, assume that (52) holds true for all trees $t = u \circ v$ of order less or equal to $n \geq 2$ (the relation $\omega(\bullet \circ \bullet) + \omega(\bullet \circ \bullet) + \omega(\bullet \times \bullet) = 2\omega(\,\dot{|}\,) + 1$ is obtained straightforwardly) and consider a tree $t = u \circ v$ of order $n + 1$: the only partition tree p^t with a skeleton of order $n + 1$ in (54) is the partition where all edges of t have been dashed. In this case, $P(p^t) = P(p^u) \cup P(p^v) = \{\bullet, \ldots, \bullet\}$, $\prod_{\delta \in P(p^t)} \gamma(\delta) = 1$, $\chi(p^u) = u$ and $\chi(p^v) = v$. Using the induction hypothesis, we obtain:

$$\omega(u \circ v) + \omega(v \circ u) + \omega(u \times v) = 0.$$

This completes the proof. □

Corollary 4.4 *Consider a B-series with coefficients a. Then the coefficients $\hat{b}$ of its modified equation satisfy:*

$$\forall (u,v) \in \mathcal{T}^2, \quad \hat{b}(u \circ v) + \hat{b}(v \circ u) = 0. \tag{56}$$

if and only if

$$\forall (u,v) \in \mathcal{T}^2, \quad a(u \circ v) + a(v \circ u) = a(u)a(v). \tag{57}$$

Remark Relation (57) characterizes symplectic methods, while relation (56) characterizes Hamiltonian fields (see Section (4.5)).

Proof

The coefficients $\hat{b}$ are given by the relation $\hat{b} = (a - \delta_e) \star \omega$. A relation similar to (55) holds with $\frac{1}{\gamma}$ replaced by a. It then follows that $\hat{b}(u \circ v) + \hat{b}(v \circ u)$ can be written as

$$\sum_{p^u, p^v} \Big(a\Big(R(p^u) \circ R(p^v) + R(p^v) \circ R(p^u)\Big)\, \omega(\chi(p^u) \times \chi(p^v)) + \omega\Big(\chi(p^u) \circ \chi(p^v) + \chi(p^v) \circ \chi(p^u)\Big)\, a(R(p^u))a(R(p^v))\Big) \prod_{\delta \in P^*(p^u) \cup P^*(p^v)} a(\delta) \quad (58)$$

and, upon using (52), further simplified to

$$\sum_{p_u, p_v} \Big(a(R(p^u) \circ R(p^v) + R(p^v) \circ R(p^u)) - a(R(p^u))a(R(p^v)) \Big) \quad \omega(\chi(p^u) \times \chi(p^v)) \prod_{\delta \in P^*(p^u) \cup P^*(p^v)} a(\delta). \quad (59)$$

If a satisfied condition (57), i.e. relation (51) for $m = 2$ with a instead of $\frac{1}{\gamma}$, then the summand of (59) vanishes. Conversely, assuming (57) for all pairs of trees (u, v) such that $|u| + |v| \leq n$, $n \geq 1$, and considering a pair with $|u| + |v| = n + 1$, it comes

$$0 = \hat{b}(u \circ v) + \hat{b}(v \circ u) = \Big(a(u \circ v) + a(v \circ u) - a(u)a(v) \Big) \quad \omega(\chi(p^u) \times \chi(p^v)) \prod_{\delta \in P^*(p^u) \cup P^*(p^v)} a(\delta) \quad (60)$$

where we have kept in the sum (59) the only non-vanishing term $(p^u, p^v) = (u, v)$ for which $(R(p^u), R(p^v)) = (u, v)$, $(\chi(p^u), \chi(p^v)) = (\bullet, \bullet)$ and $(P^*(p^u), P^*(p^v)) = (\emptyset, \emptyset)$. Since $\omega(\bullet) = 1$, this simply gives

$$0 = a(u \circ v) + a(v \circ u) - a(u)a(v)$$

and the stated result follows by induction. □

Now, we can elaborate the following generalization of (52):

Proposition 4.5 *The coefficients ω of the modified equation of the explicit Euler method satisfy the following relation for all triplets of trees $(u, v, w) \in \mathcal{T}^3$:*

$$\omega(u \circ v \circ w) + \omega(v \circ u \circ w) + \omega(v \circ u \circ w) + \omega(u \times v \times w) + \omega(u \times v \circ w) + \omega(v \times w \circ u) + \omega(w \times u \circ v) = 0. \quad (61)$$

Proof

We can follow step by step the proof of Proposition 4.3. The tableau corresponding to the situation of a tree $t = u \circ v \circ w$ becomes:

p^t	$\chi(p^t)$	$P(p^t)$
$p^u \circ p^v \circ p^w$	$\chi(p^u) \times \chi(p^v) \times \chi(p^w)$	$P^*(p^u) \cup P^*(p^v) \cup P^*(p^w) \cup \{R(p^u) \circ R(p^v) \circ R(p^w)\}$
$p^u \bullet p^v \circ p^w$	$\chi(p^u) \circ \chi(p^v) \times \chi(p^w)$	$P^*(p^u) \cup P^*(p^v) \cup P^*(p^w) \cup \{R(p^u) \circ R(p^w),\ R(p^v)\}$
$p^u \circ p^v \bullet p^w$	$\chi(p^u) \times \chi(p^v) \circ \chi(p^w)$	$P^*(p^u) \cup P^*(p^v) \cup P^*(p^w) \cup \{R(p^u) \circ R(p^v),\ R(p^w)\}$
$p^u \bullet p^v \bullet p^w$	$\chi(p^u) \circ \chi(p^v) \circ \chi(p^w)$	$P^*(p^u) \cup P^*(p^v) \cup P^*(p^w) \cup \{R(p^u),\ R(p^v),\ R(p^w)\}$

(62)

Hence, in the expression of $\Big((\frac{1}{\gamma} - \delta_e) \star \omega\Big)(u \circ v \circ w + v \circ u \circ w + w \circ u \circ v)$ the term $\omega(\chi(p^u) \times \chi(p^v) \times \chi(p^w))$ has a factor

$$\Big(\frac{1}{\gamma}\Big)(R(p^u) \circ R(p^v) \circ R(p^w) + R(p^v) \circ R(p^u) \circ R(p^w) + R(p^w) \circ R(p^u) \circ R(p^v)) \prod_{\delta \in P^*(p^u) \cup P^*(p^v) \cup P^*(p^w)} \frac{1}{\gamma(\delta)}, \quad (63)$$

and the terms $\omega(\chi(p^u) \circ \chi(p^v) \circ \chi(p^w))$, $\omega(\chi(p^v) \circ \chi(p^u) \circ \chi(p^w))$ and $\omega(\chi(p^w) \circ \chi(p^u) \circ \chi(p^v))$ all have a factor

$$\prod_{\delta \in P(p^u) \cup P(p^v) \cup P(p^w)} \frac{1}{\gamma(\delta)}.$$

There remain six terms which can be gathered by pairs, owing the fact that for any three trees t_1, t_2, s, one has:

$$t_1 \times t_2 \circ s = t_1 \circ s \times t_2 = t_2 \circ s \times t_1 = t_2 \times t_1 \circ s.$$

Hence, the term $\omega(\chi(p^u)\times\chi(p^w)\circ\chi(p^v))$ has a factor

$$\Big(\frac{1}{\gamma}\Big)(R(p^u)\circ R(p^w)+R(p^w)\circ R(p^u))\prod_{\delta\in P^*(p^u)\cup P(p^v)\cup P^*(p^w)}\frac{1}{\gamma(\delta)},$$

the term $\omega(\chi(p^u)\times\chi(p^v)\circ\chi(p^w))$ has a factor

$$\Big(\frac{1}{\gamma}\Big)(R(p^u)\circ R(p^v)+R(p^v)\circ R(p^u))\prod_{\delta\in P^*(p^u)\cup P^*(p^v)\cup P(p^w)}\frac{1}{\gamma(\delta)},$$

and the term $\omega(\chi(p^v)\times\chi(p^w)\circ\chi(p^u))$ has a factor

$$\Big(\frac{1}{\gamma}\Big)(R(p^v)\circ R(p^w)+R(p^w)\circ R(p^v))\prod_{\delta\in P(p^u)\cup P^*(p^v)\cup P^*(p^w)}\frac{1}{\gamma(\delta)}.$$

Using relation (51) with $m=2$ and $m=3$, it can be seen that all factors turn out to be equal to

$$\prod_{\delta\in P(p^u)\cup P(p^v)\cup P(p^w)}\frac{1}{\gamma(\delta)}.$$

Denoting μ the function defined on triplets of trees by:

$$\mu(t_1,t_2,t_3)=\omega\Big(t_1\circ t_2\circ t_3+t_2\circ t_1\circ t_3+t_3\circ t_1\circ t_2+t_1\times t_2\times t_3+t_1\times t_2\circ t_3+t_2\times t_3\circ t_1+t_3\times t_1\circ t_2\Big),$$

we finally get the equation

$$\Big((\frac{1}{\gamma}-\delta_e)\star\omega\Big)(u\circ v\circ w+v\circ u\circ w+w\circ u\circ v)=\sum_{p^u,\,p^v,\,p^w}\mu(\chi(p^u),\chi(p^v),\chi(p^w))\prod_{\delta\in P(p^u)\cup P(p^v)\cup P(p^w)}\frac{1}{\gamma(\delta)}.\quad(64)$$

The same induction as in Proposition (4.3) leads to the result ((61) for the third-order tree $t=\bullet\circ\bullet\circ\bullet$ is obtained directly). ☐

Corollary 4.6 *Consider a B-series with coefficients a. The following condition*

$$\forall(u,v,w)\in\mathcal{T}^3,\quad a(u\circ v\circ w)+a(v\circ u\circ w)+a(w\circ u\circ v)=a(u)a(v)a(w)\quad(65)$$

holds if and only if the coefficients $\hat{b}$ *of its modified equation satisfy:*

$$\forall(u,v,w)\in\mathcal{T}^3,\quad \hat{b}(u\circ v\circ w)+\hat{b}(v\circ u\circ w)+\hat{b}(w\circ u\circ v)=0.\quad(66)$$

Conditions (65) characterize integrators that preserve cubic polynomials. It is proved in [CFM05] that there exists no integrator that preserves all polynomial invariants of degree less than 3. Finally, we end up by giving the full generalization of Proposition 4.3:

Proposition 4.7 *The coefficients* ω *of the modified equation of the explicit Euler method satisfy the following relation for all m-uplets of trees* $(u_1,\ldots,u_m)\in\mathcal{T}^m$*:*

$$\sum_{i=1}^{m}\ \sum_{1\le j_1<j_2<\ldots<j_i\le m}\omega\Big(\times_{l=1}^{i}u_{j_l}\circ\prod_{l=i+1}^{m}u_{j_l}\Big)=0.\quad(67)$$

Corollary 4.8 *Consider a B-series with coefficients a satisfying the condition:*

$$\forall m,\ 2\le m\le n,\quad\forall(u_1,\ldots,u_m)\in\mathcal{T}^m,\quad\sum_{i=1}^{m}a(u_i\circ\prod_{j\neq i}u_j)=\prod_{i=1}^{m}a(u_i).\quad(68)$$

Then the coefficients $\hat{b}$ *of its modified equation satisfy:*

$$\forall m,\ 2\le m\le n,\quad\forall(u_1,\ldots,u_m)\in\mathcal{T}^m,\quad\sum_{i=1}^{m}b(u_i\circ\prod_{j\neq i}u_j)=0.\quad(69)$$

The converse is also true.

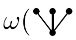
If we take $u_1 = u_2 = \ldots = u_m = \bullet$, relation (67) becomes:

$$\sum_{i=1}^{m} \frac{m!}{i!(m-i)!} \omega([\bullet^{m-i}]) = 0. \tag{70}$$

Since $\omega(\bullet) = 1$, this shows that

$$\omega([\bullet^{i}]) = B_i \tag{71}$$

where the B_i's are the Bernoulli numbers. Hence, we have

$\omega($  $) = B_1 = -1/2, \quad \omega($  $) = B_2 = 1/6, \quad \omega($  $) = B_3 = 0, \ldots$

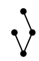
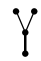
τ	e	$\bullet$							
$\omega(\tau)$	0	1	$-\frac{1}{2}$	$\frac{1}{6}$	$\frac{1}{3}$	$-\frac{1}{12}$	$-\frac{1}{6}$	$-\frac{1}{4}$	0

Table 7: Coefficients $\omega(\tau)$ appearing in (49),(50) for trees of order ≤ 4.

4.2 Generating function methods

The idea of generating function methods is that the exact solution of $\dot{y} = f(y)$, can be interpreted as the numerical solution of a modified differential equation $\dot{\breve{y}} = \breve{f}(\breve{y})$, using the numerical method $\Phi_h^{\breve{f}}$:

Theorem 4.9 *There exists a modified field* $\breve{f}(y) = \breve{f}_1(y) + h\breve{f}_2(y) + h^2\breve{f}_3(y) + \ldots$ *such as*

$$\Phi_h^{\breve{f}}(y_0) = y(h),$$

where $y(t)$ *denotes the exact solution of*

$$\begin{cases} \dot{y} &= f(y) \\ y(0) &= y_0 \end{cases}.$$

Moreover, $\breve{f}(y)$ *is defined by*

$$h\breve{f}(y) = B_f(\breve{b}, y),$$

where $\breve{b} \in \mathsf{Fields}$ *is the solution of*

$$\breve{b} \star a = \frac{1}{\gamma}. \tag{72}$$

Remark If one truncates the field $\breve{f}(y)$ at order p, by taking

$$\breve{f}(y) = \breve{f}_1(y) + h\breve{f}_2(y) + h^2\breve{f}_3(y) + \ldots + h^{p-1}\breve{f}_p(y),$$

then the numerical methods obtained by using this truncated field instead of $f(y)$ has order (at least) p.

Proof of Theorem 4.9
We have

$$\Phi_h^{\breve{f}}(y_0) = B_{\breve{f}}(a, y) = B_f(\breve{b} \star a, y),$$

and

$$y(h) = B_f(\frac{1}{\gamma}, y_0).$$

We conclude like in the proof of Theorem 4.1.

modified equation for backward error analysis *(Theorem 4.1)*	$\begin{cases} \dot{\hat{y}} = \hat{f}(\hat{y}) \\ \hat{y}(0) = y_0 \end{cases}$	
		$\searrow$ exact solution: $\hat{y}(nh) = y_n$
		$y_{n+1} = \Phi_h^f(y_n)$
		$\nearrow$ numerical solution: $y(nh) \approx y_n$
initial problem (1)	$\begin{cases} \dot{y} = f(y) \\ y(0) = y_0 \end{cases}$	
		$\searrow$ exact solution: $y(nh) = \breve{y}_n$
		$\breve{y}_{n+1} = \Phi_h^{\breve{f}}(\breve{y}_n)$
		$\nearrow$ numerical solution: $\breve{y}(nh) \approx \breve{y}_n$
modified equation for generating function methods *(Theorem 4.9)*	$\begin{cases} \dot{\breve{y}} = \breve{f}(\breve{y}) \\ \breve{y}(0) = y_0 \end{cases}$	

Table 8: A link between backward error analysis and generating function methods

4.3 A link between backward error analysis and generating function methods

Substituting the expression of $\frac{1}{\gamma}$ given in (72) into (48) gives $\hat{b} \star \breve{b} \star a = a$. Therefore $\breve{b}$ and $\hat{b}$ are inverse elements for substitution law $\star$:

$$\hat{b} \star \breve{b} = \breve{b} \star \hat{b} = \delta_{\bullet}. \tag{73}$$

This can be interpreted through Table 8, by saying that backward error analysis and generating function methods are opposite procedures.

4.4 Adjoint methods, symmetric methods

Theorem 4.10 *Let $\hat{b}^*$ and $\breve{b}^*$ denote the modified field coefficients given in Theorems 4.1 and 4.9, and corresponding to the adjoint method $\Phi_h^*(y) = B(a^*, y)$ of $\Phi_h(y) = B(a, y)$.*
Then, for all $\tau \in \mathcal{T}$,

$$\hat{b}^*(\tau) = (-1)^{|\tau|+1}\hat{b}(\tau), \tag{74}$$
$$\breve{b}^*(\tau) = (-1)^{|\tau|+1}\breve{b}(\tau). \tag{75}$$

Proof of Theorem 4.10

Result (74) can be found in [HLW02], IX.2, Theorem 2.1, p. 292. It is equivalent to

$$\hat{b}^* = (-\delta_{\bullet}) \star \hat{b} \star (-\delta_{\bullet}). \tag{76}$$

Using relation (76), we may now prove (75). For substitution law $\star$, the inverse of $\hat{b}$ is $\breve{b}$, the inverse of $\hat{b}^*$ is $\breve{b}^*$, and $-\delta_{\bullet}$ is its own inverse. Therefore, inverting relation (76) for $\star$ law yields

$$\breve{b}^* = (-\delta_{\bullet}) \star \breve{b} \star (-\delta_{\bullet}), \tag{77}$$

which is equivalent to (75). □

Remark It may be interesting to get (74) using the algebraic properties of substitution law $\star$. We use

$$a^* = (-\delta_{\bullet}) \star a^{-1}. \tag{78}$$

Because the exact flow is symmetric, we have

$$\left(\frac{1}{\gamma}\right)^{-1} = -\delta_{\bullet} \star \frac{1}{\gamma}. \tag{79}$$

Then,

$$a^* \overset{(78)}{=} (-\delta_\bullet)\star a^{-1} \overset{(48)}{=} (-\delta_\bullet)\star(\hat{b}\star\frac{1}{\gamma})^{-1} \overset{(43)}{=} (-\delta_\bullet)\star\hat{b}\star(\frac{1}{\gamma})^{-1} \overset{(79)}{=} (-\delta_\bullet)\star\hat{b}\star(-\delta_\bullet)\star\frac{1}{\gamma}. \tag{80}$$

Therefore, Theorem 4.9 gives (74).

We can notice that the same method also works to prove (75):

$$\frac{1}{\gamma} \overset{(79)}{=} (-\delta_\bullet)\star(\frac{1}{\gamma})^{-1} \overset{(72)}{=} (-\delta_\bullet)\star(\breve{b}\star a)^{-1} \overset{(43)}{=} (-\delta_\bullet)\star\breve{b}\star a^{-1} \overset{(78)}{=} (-\delta_\bullet)\star\breve{b}\star(-\delta_\bullet)\star a^*. \tag{81}$$

For symmetric methods, we then have the following result.

Definition 4.11 *We define the subset* Sym *of symmetric mappings*

$$\begin{aligned} \mathsf{Sym} &= \{b\in\mathsf{Fields}\ ;\ b=(-\delta_\bullet)\star b\star(-\delta_\bullet)\} \\ &= \{b\in\mathsf{Fields}\ ;\ b(\tau)=0 \textit{ whenever } |\tau| \textit{ is even}\}, \end{aligned} \tag{82}$$

where the set Fields *is given in definition 3.3.*

Theorem 4.12 Sym *is a subgroup of* Fields *for substitution law* $\star$.

Theorem 4.13 *Moreover, method* $\Phi_h(y)=B(a,y)$ *is symmetric (i.e.* $\Phi_h^*=\Phi_h$*) if and only if* $\hat{b},\breve{b}\in\mathsf{Sym}$*, where* $\hat{b}$ *and* $\breve{b}$ *are the modified field coefficients given in Theorems 4.1 and 4.9.*

4.5 Hamiltonian fields and symplectic methods

4.5.1 Hamiltonian fields: a subgroup

Definition 4.14 *We define the set* Ham *of mappings by*

$$\mathsf{Ham}=\{b\in\mathsf{Fields}\ ;\ \forall u,v\in\mathcal{T},\ b(u\circ v)+b(v\circ u)=0\}, \tag{83}$$

where the set Fields *is given in definition 3.3, and the Butcher product* $u\circ v$ *is given in definition 2.7.*

The set Ham is the set of mappings corresponding to Hamiltonian fields, according to the following result.

Theorem 4.15 ***(Hairer, [Hai94]).***
Let $b\in\mathsf{Fields}$*. Consider the (h-dependent) field* $g:\mathbb{R}^d\to\mathbb{R}^d$ *defined by*

$$hg(y)=B_f(b,y).$$

Then, g(y) is a Hamiltonian field for all $f(y)=J^{-1}\nabla H(y)$ *if and only if* $b\in\mathsf{Ham}$*.*

Then we have the following result.

Theorem 4.16 *The set* Ham *is a subgroup of* Fields *for substitution law* $\star$.

To prove Theorem 4.16 we need the following two propositions.

Proposition 4.17 *Let* $b,c\in\mathsf{Ham}$*. Then* $b\star c\in\mathsf{Ham}$*.*

Proof of Proposition 4.17
The field $B_g(c,y)$ is Hamiltonian for all Hamiltonian field $g(y)$, and in particular for $hg(y)=B_f(b,y)$. □

Proposition 4.18 *Let* $b,c\in\mathsf{Fields}$*, satisfying* $c\star b\in\mathsf{Ham}$*. Then,* $b\in\mathsf{Ham}$ *if and only if* $c\in\mathsf{Ham}$*.*

Proof of Proposition 4.18
Let $c\in\mathsf{Ham}$. Like in the proof of Theorem IX.10.1, p. 320 in [HLW02], consider the truncation mappings $b_N\in\mathsf{Fields}$ defined for all $N\geq 1$ by

$$\forall\tau\in\mathcal{T},\ b_N(\tau)=\begin{cases} b(\tau) \text{ if } |\tau|\leq N, \\ 0 \text{ if } |\tau|>N. \end{cases} \tag{84}$$

We then show that $b_N \in \mathsf{Ham}$ by induction on N. The result is clear for $N = 1$. For $N > 1$, suppose that $b_{N-1} \in \mathsf{Ham}$.

For $\tau \in \mathcal{T}$ with $|\tau| = N$, using formula (28), we get

$$b_N(\tau)c(\bullet)^{|\tau|} = c \star b(\tau) - c \star b_{N-1}(\tau). \tag{85}$$

Since $b_{N-1}, c \in \mathsf{Ham}$, Proposition 4.17 gives $c \star b_{N-1} \in \mathsf{Ham}$. Moreover $c(\bullet) \neq 0$, and $c \star b \in \mathsf{Ham}$ by assumption. Therefore, for all $u, v \in \mathcal{T}$ with $|u| + |v| = N$,

$$b_N(u \circ v) + b_N(v \circ u) = 0.$$

We get $b_N \in \mathsf{Ham}$ for all $N \geq 1$, i.e. $b \in \mathsf{Ham}$.

Reciprocally, if $b \in \mathsf{Ham}$, to prove $c \in \mathsf{Ham}$, we use the similar relation

$$\text{for } |\tau| = N,\ b(\bullet)c_N(\tau) = c \star b(\tau) - c_{N-1} \star b(\tau). \tag{86}$$

□

Remark One can also prove previous propositions (4.17) and (4.18) by induction using formula (58) with b instead of ω and c instead of $a - \delta_e$.

Proof of Theorem 4.16

Unit element $\delta_\bullet$ is in Ham, and Proposition 4.17 is satisfied. Moreover, for $c \in \mathsf{Ham}$, if b denotes the inverse of c for $\star$, we have $c \star b = \delta_\bullet \in \mathsf{Ham}$, and therefore, Proposition 4.18 gives $c \in \mathsf{Ham}$. □

4.5.2 Symplectic methods

In this section we give the following result.

Theorem 4.19 *If a symplectic method $\Phi_h(y)$ is applied to a (smooth) Hamiltonian system, then the modified field $\breve{f}(y)$, defined in Theorem 4.9, as well as $\hat{f}(y)$ defined in Theorem 4.1, is also Hamiltonian.*

More precisely, we will prove Theorem 4.22.

Definition 4.20 *We define the set* Sympl *of mappings by*

$$\mathsf{Sympl} = \{a : \mathcal{T} \cup \{e\} \to \mathbb{R}\ ;\ a(e) = 1,\ \forall u, v \in \mathcal{T},\ a(u \circ v) + a(v \circ u) = a(u)a(v)\}. \tag{87}$$

The set Sympl is the set of mappings corresponding to symplectic methods according to the following result.

Theorem 4.21 ***(Calvo & Sanz-Serna, [CSS94], see also [HLW02], VI.7)***

The numerical method $\Phi_h^f(y) = B_f(a, y)$ is symplectic for all $f(y) = J^{-1}\nabla H(y)$ if and only if $a \in \mathsf{Sympl}$.

Theorem 4.22 *Let $a : \mathcal{T} \cup \{e\} \to \mathbb{R}$ be a mapping satisfying $a(e) = 1$, $a(\bullet) \neq 0$.*
Then, the following assertions are equivalent:

(i) $a \in \mathsf{Sympl}$,

(ii) $\hat{b} \in \mathsf{Ham}$, *where $\hat{b}$ is defined in Theorem 4.1 (backward error analysis),*

(iii) $\breve{b} \in \mathsf{Ham}$, *where $\breve{b}$ is defined in Theorem 4.9 (generating function methods).*

Proof of Theorem 4.22

Implication $(i) \Rightarrow (ii)$ corresponds to Theorem IX.3.1, pages 293-294 in [HLW02]. It is also proved 'algebraically' in Corollary 4.4.
Equivalence $(ii) \Leftrightarrow (iii)$ comes from the fact that Ham is a subgroup of Fields (Theorem 4.16) and (73).

Finally, $(ii) \Rightarrow (i)$ is immediate, since $\frac{1}{\gamma} \in \mathsf{Sympl}$ together with $\hat{b} \in \mathsf{Ham}$ implies $a = \hat{b} \star \frac{1}{\gamma} \in \mathsf{Sympl}$. □

Remark Indeed, a symplectic method applied with a Hamiltonian field gives a symplectic method, i.e., for $a \in \mathsf{Sympl}$, $b \in \mathsf{Ham}$, we have $b \star a \in \mathsf{Sympl}$.

More generally, we mention the following result, which is a consequence of Theorems 4.16 and 4.22.

Corollary 4.23 *Let* $a : \mathcal{T} \cup \{e\} \to \mathbb{R}$ *be a mapping satisfying* $a(e) = 1$, $a(\bullet) \neq 0$, *and* $b \in \mathsf{Fields}$. *Consider the following assertions:*

1. $a \in \mathsf{Sympl}$,
2. $b \in \mathsf{Ham}$,
3. $b \star a \in \mathsf{Sympl}$.

If two of the above three assertions are satisfied, then the third one is also satisfied. In other words, we have (1 *and* 2) $\Rightarrow$ 3, (2 *and* 3) $\Rightarrow$ 1, (1 *and* 3) $\Rightarrow$ 2.

Proof of Corollary 4.23

First, we prove (2 and 3) $\Rightarrow$ 1. Because of Theorem 4.16, for $b \in \mathsf{Ham}$, there exists $c \in \mathsf{Ham}$ satisfying $c \star b = \delta_{\bullet}$. Then, $a = \delta_{\bullet} \star a = c \star (b \star a)$, whence $a \in \mathsf{Sympl}$ because $b \star a \in \mathsf{Sympl}, c \in \mathsf{Ham}$.

Finally, we prove (1 and 3) $\Rightarrow$ 2. For $a \in \mathsf{Sympl}$, Theorem 4.22 gives $a = \hat{b} \star \frac{1}{\gamma}$ where $\hat{b} \in \mathsf{Ham}$. Then $(\hat{b} \star b) \star \frac{1}{\gamma} = b \star a \in \mathsf{Sympl}$. Therefore, using Theorem 4.22 again, $b \star \hat{b} \in \mathsf{Ham}$. Because $\hat{b} \in \mathsf{Ham}$, Theorem 4.16 gives $b \in \mathsf{Ham}$. □

References

[Bro04] Ch. Brouder. Trees, renormalization and differential equations. *BIT*, 44(3):425–438, 2004.

[But69] J. C. Butcher. The effective order of Runge-Kutta methods. In J. Ll. Morris, editor, *Proceedings of Conference on the Numerical Solution of Differential Equations*, volume 109 of *Lecture Notes in Math.*, pages 133–139, 1969.

[But72] J. C. Butcher. An algebraic theory of integration methods. *Math. Comput.*, 26:79–106, 1972.

[CFM05] P. Chartier, E. Faou, and A. Murua. An algebraic analysis of formal methods preserving structures. *in preparation*, 2005.

[CK98] A. Connes and D. Kreimer. Hopf algebras, renormalization and noncommutative geometry. *Commun. Math. Phys.*, 199, 1998.

[CL98] P. Chartier and E. Lapôtre. Reversible B-series. *INRIA report*, 1998. No. 1221.

[CMSS94] M. P. Calvo, A. Murua, and J. M. Sanz-Serna. Modified equations for ODEs. *Contemporary Mathematics*, 172:63–74, 1994.

[CS90] P. J. Channell and J. C. Scovel. Symplectic integration of Hamiltonian systems. *Nonlinearity*, 3:231–259, 1990.

[CSS94] M. P. Calvo and J. M. Sanz-Serna. Canonical B-series. *Numer. Math.*, 67:161–175, 1994.

[Fen86] K. Feng. Difference schemes for Hamiltonian formalism and symplectic geometry. *J. Comp. Math.*, 4:279–289, 1986.

[FWQW89] K. Feng, H. M. Wu, M.-Z. Qin, and D. L. Wang. Construction of canonical difference schemes for Hamiltonian formalism via generating functions. *J. Comp. Math.*, 7:71–96, 1989.

[Hai94] E. Hairer. Backward analysis of numerical integrators and symplectic methods. *Annals of Numerical Mathematics*, 1:107–132, 1994.

[Hai99] E. Hairer. Backward error analysis for multistep methods. *Numer. Math.*, 84:199–232, 1999.

[HLW02] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations.* Springer Series in Computational Mathematics 31. Springer, Berlin, 2002.

[HW74] E. Hairer and G. Wanner. On the Butcher group and general multi-value methods. *Computing*, 13:1–15, 1974.

[Mur03] A. Murua. The Hopf algebra of rooted trees, free Lie algebras, and Lie series. *Submitted*, 2003.

Contents

Unité de recherche INRIA Rennes
IRISA, Campus universitaire de Beaulieu - 35042 Rennes Cedex (France)

Unité de recherche INRIA Futurs : Domaine de Voluceau - Rocquencourt - BP 105 - 78153 Le Chesnay Cedex (France)
Unité de recherche INRIA Lorraine : LORIA, Technopôle de Nancy-Brabois - Campus scientifique
615, rue du Jardin Botanique - BP 101 - 54602 Villers-lès-Nancy Cedex (France)
Unité de recherche INRIA Rhône-Alpes : 655, avenue de l'Europe - 38330 Montbonnot-St-Martin (France)
Unité de recherche INRIA Rocquencourt : Domaine de Voluceau - Rocquencourt - BP 105 - 78153 Le Chesnay Cedex (France)
Unité de recherche INRIA Sophia Antipolis : 2004, route des Lucioles - BP 93 - 06902 Sophia Antipolis Cedex (France)

Éditeur
INRIA - Domaine de Voluceau - Rocquencourt, BP 105 - 78153 Le Chesnay Cedex (France)
http://www.inria.fr
ISSN 0249-6399