

Preserving first integrals and volume forms of additively split systems

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*Preserving first integrals and volume forms of
additively split systems*

Philippe Chartier and Ander Murua

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Preserving first integrals and volume forms of additively split systems

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Abstract: This work is concerned with the preservation of invariants and of volume-forms by numerical methods which can be expanded into B-series. The situation we consider here is that of a split vector field $f = f^{[1]} + \dots + f^{[N]}$ where each $f^{[v]}$ either has the common invariant I or is divergence free. We derive algebraic conditions on the coefficients of the B-series for it either to preserve I or to preserve the volume for generic vector fields and interpret them for additive Runge-Kutta methods. Comparing the two sets of conditions then enables us to state some non-existence results. For a more restrictive class of problems, where the system is partitionned into several components, we nevertheless obtain simplified conditions and show that they can be solved.

Key-words: polynomial invariants, volume-form, split systems, B-series, S-series

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Intégrateurs numériques préservant les invariants et/ou la forme volume

Résumé : Cet article traite de la préservation des invariants et de la forme volume attachés à un système d'équations différentielles par une méthode numérique représentable en B-series.

Mots-clés : invariants polynomiaux, forme volume, systèmes partitionnés, B-séries, S-séries

Contents

1	Introduction	3
2	Basic tools	5
2.1	The algebra of trees	5
2.2	B-series, S-series and their composition	6
3	Preservation of exact invariants	8
4	Volume preserving integrators	12
4.1	Divergence-free B-series	12
4.1.1	Aromatic trees	12
4.1.2	Divergence-free conditions and first consequences	15
4.2	Volume-preserving B-series	16
4.2.1	Conditions for additive Runge-Kutta methods	18
4.3	Systems with additional structure	20
4.3.1	Hamiltonian systems	20
4.3.2	Two-cycles systems	21
4.3.3	Three-cycles systems	23

1 Introduction

Preserving volume forms is a necessary requirement in several well-identified applications, such as molecular dynamics or meteorology, while preserving first integrals is vastly recognized as fundamental in a very large number of physical situations. Although the requirements appear somehow disconnected, they lead to algebraic conditions which have strong similarities and this is the very reason why we address these questions together.

We will show in particular that a method that preserves the volume must also preserve all first integrals¹ and as a consequence, that no volume-preserving B-series method exists apart from the composition of exact flows (see Theorem 6 of Section 4.2). This result generalizes to split vector fields a known result of Feng Kang and Shang Zai-jui [FS95]. Let us notice that a similar result, using rather different techniques of proof, has been derived independently by Tse, Iserles and Quispel [TIQ06]. A noticeable difference is in particular that we obtain conditions on both the modified vector-field (which has to be divergence-free) and the method itself (which is volume-preserving): this then allows for the derivation of algebraic conditions set directly on the coefficients of an additive Runge-Kutta method (see Section 4.2.1).

¹The fact that no Runge-Kutta method can preserve polynomial invariants of degree less or equal to 3 was first shown by Calvo, Iserles and Zanna in [CIZ97] and the extension of this result to arbitrary degree was considered in [Zan98, IZ00]. Here, we extend this result to arbitrary B-series for split vector fields.

It is however interesting to consider specific classes of problems, for which volume-preserving integrators can be constructed. For instance, it is clear that symplectic methods are volume-preserving for Hamiltonian systems: in Section 4.3.1, we show that symplectic conditions are in general necessary for a method to be volume-preserving and indeed sufficient for the special class of Hamiltonian problems. In a similar spirit, we derive in Section 4.3 simplified conditions for partitioned systems with two functions and three functions. The results obtained for two functions corroborate already known ones (see Theorem 3.4. of [HLW02]) and results for more than three functions (and their straightforward generalization to more functions) appear to be completely new. It is interesting to notice that the general idea used here to obtain numerical methods also has some similarities with the technique considered by H. Munthe-Kass, A. Iserles, R. Quispel and A. Zanna [IMKQZ06] for polynomial vector fields.

In the sequel, we shall thus consider a n -dimensional system of differential equations of the form

$$\dot{y}(x) = \sum_{v=1}^N f^{[v]}(y), \quad (1.1)$$

$$= f^{[1]}(y) + f^{[2]}(y) + \dots + f^{[N]}(y). \quad (1.2)$$

A NB-series $NB(a)$ is a formal expression of the form

$$NB(a) = id_{\mathbb{R}^n} + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} a(t) F(t), \quad (1.3)$$

where the index set \mathcal{T} is the set of N -coloured rooted trees, $|\cdot|$, σ and F are real functions defined on \mathcal{T} and where a is a function defined on \mathcal{T} as well which characterizes the NB-series itself. These series have been introduced in [AMSS97] in full details for the purpose of studying symplectic additive Runge-Kutta methods. Note that this definition coincides with the standard definition of B-series as given in [HLW02] when only one colour is used for the vertices. In the sequel, we shall simply write $B(a)$ for the general case, and refer NB-series as B-series.

As in [CFM06], S-series arise naturally: in accordance with B-series, we consider here S-series for coloured trees. For instance, for $N = 2$, and for a smooth function g , a S-series is a series of the form

$$\begin{aligned} S(\alpha)[g] &= \alpha(e)g + h\alpha(\bullet)g_y f^{[1]} + h\alpha(\circ)g_y f^{[2]} \\ &\quad + h^2 \left(\frac{\alpha(\bullet\bullet)}{2} g_{yy}(f^{[1]}, f^{[1]}) + \alpha(\bullet\circ)g_{yy}(f^{[1]}, f^{[2]}) + \frac{\alpha(\circ\circ)}{2} g_{yy}(f^{[2]}, f^{[2]}) \right) \\ &\quad + h^2 \left(\alpha(\curvearrowright)g_y f_y^{[1]} f^{[1]} + \alpha(\curvearrowleft)g_y f_y^{[1]} f^{[2]} + \alpha(\curvearrowright)g_y f_y^{[2]} f^{[1]} + \alpha(\curvearrowleft)g_y f_y^{[2]} f^{[2]} \right) + \dots \end{aligned}$$

Assuming that a function I with a S-series expansion is a first integral of individual differential equations $\dot{y} = f^{[v]}(y)$, $v = 1, \dots, N$, i.e. satisfies

$$\forall v = 1, \dots, N, \forall y \in \mathbb{R}^n, \left(\nabla I(y) \right)^T f^{[v]}(y) = 0, \quad (1.4)$$

preserving I for an integrator $B(a)$ amounts to satisfying the condition

$$\forall y \in \mathbb{R}^n, \left(I \circ B(a) \right) (y) = I(y),$$

and it can be shown [Mur99], that

$$I \circ B(a) = S(\alpha)[I], \tag{1.5}$$

where α , acting on \mathcal{F} , is uniquely defined in terms of a . All further results of this paper will be obtained in this framework.

2 Basic tools

In this first section, we describe very briefly the basic algebraic tools that allow for the manipulation of S-series. Since the definitions used here are rather similar to [CFM06], we shall focus mainly on the differences with the one-colour situation.

2.1 The algebra of trees

Definition 1 (Rooted trees, Forests) *The set of (rooted) trees \mathcal{T} and forests \mathcal{F} are defined recursively by:*

1. *the forest e is the empty forest*
2. *if t_1, \dots, t_n are n trees of \mathcal{T} , the forest $u = t_1 \dots t_n$ is the commutative juxtaposition of t_1, \dots, t_n*
3. *if u is a forest of \mathcal{F} , then $t = [u]_v$, where $v \in \{1, \dots, N\}$ is a tree of \mathcal{T} with root of colour v .*

The order of a tree is its number of vertices and is denoted by $|t|$. The order $|u|$ of a forest $u = t_1 \dots t_n$ is the sum of the $|t_i|$'s. If $u = t_1^{r_1} \dots t_n^{r_n}$ where t_1, \dots, t_n are pairwise distinct and are repeated respectively r_1, \dots, r_n times, then the symmetry σ of u is

$$\sigma(u) = r_1! \dots r_n! (\sigma(t_1))^{r_1} \dots (\sigma(t_n))^{r_n}.$$

By convention, $\sigma(e) = 1$. The symmetry $\sigma(t)$ of a tree $t = [u]_v$ is the symmetry of u . The set of linear combinations of forests in \mathcal{F} can be naturally endowed with an algebra structure \mathcal{H} and the tensor product of \mathcal{H} with itself can be defined just as in [CFM06]. We will further denote by $\text{Alg}(\mathcal{H}, \mathbb{R})$ the space of algebra morphisms from \mathcal{H} to \mathbb{R} and by \mathcal{H}^* the space of linear forms on \mathcal{H} . Eventually, the co-product has to take into account the possibility of trees with different colours: hence, the operator B^+ becomes B_v^+ as defined below:

$$B_v^+ : \begin{array}{ccc} \mathcal{F} & \rightarrow & \mathcal{T} \\ u = t_1 \dots t_n & \mapsto & [t_1 \dots t_n]_v \end{array}$$

Example 1

$$B_1^+(\bullet \circ) = \left[\bullet \circ \right]_1 = \mathfrak{V} \text{ and } B^-(\mathfrak{V}\bullet) = \bullet \bullet \bullet$$

Defining $\mu(t)$ as the colour of the root of t , we then have:

Definition 2 (Co-product) The co-product Δ is a **linear** map from \mathcal{H} to $\mathcal{H} \otimes \mathcal{H}$ defined recursively by:

1. $\Delta(e) = e \otimes e$,
2. $\forall t \in \mathcal{T}, \Delta(t) = t \otimes e + (id_{\mathcal{H}} \otimes B_{\mu(t)}^+) \circ \Delta \circ B^-(t)$,
3. $\forall u = t_1 \dots t_n \in \mathcal{F}, \Delta(u) = \Delta(t_1) \dots \Delta(t_n)$.

Remark 1 The co-product of a tree can also be written as (see [CK98] for instance)

$$\Delta(t) = t \otimes e + \sum_i u_i \otimes s_i, \quad (2.1)$$

where $s_i \in \mathcal{T}$ is a subtree of t and u_i the forest obtained when removing s_i from t .

2.2 B-series, S-series and their composition

For a tree $t \in \mathcal{T}$ the elementary differential $F^{[v]}(t)$ is a mapping from \mathbb{R}^n to \mathbb{R}^n , defined recursively by:

$$F(\bullet_v)(y) = f^{[v]}(y), \quad F([t_1 \dots t_n]_v)(y) = \frac{\partial^n f^{[v]}}{\partial y^n}(y) \left(F(t_1)(y), \dots, F(t_n)(y) \right),$$

where $\bullet_v = [e]_v$.

Differential operators associated to a forest and S-series are exactly the same as for the one-colour situation, and we refer to [CFM06] for the formal definitions.

Example 2 For $g \in \mathcal{D}$, one has

$$X(e)[g] = g, \quad X(\bullet_v)[g] = g_y f^{[v]}, \quad X(\mathfrak{J})[g] = g_y f_y^{[1]} f^{[2]}, \quad X(\mathfrak{J} \bullet \circ) = g_{yyy} \left(f_y^{[2]} f^{[1]}, f^{[1]}, f^{[2]} \right).$$

More generally, the relations

$$X(t)[id_{\mathbb{R}^n}] = F(t), \quad X(u)[f^{[v]}] = F([u]_v),$$

hold true.

Now, considering the action of a map $g \in \mathcal{D}$ on a B-series $B(a)$, the following formula can be obtained [Mur99]:

$$g \circ B(a) = \sum_{u \in \mathcal{F}} \frac{h^{|u|}}{\sigma(u)} \alpha(u) X(u)[g], \quad (2.2)$$

with $\alpha(e) = 1$ and $\alpha(t_1 \dots t_j) = a(t_1) \dots a(t_j)$. It follows that to every B-series $B(a)$ can be associated a S-series $S(\alpha)$ where α is an algebra morphism

Lemma 1 (Composition of S-series) *Let α and β be in \mathcal{H}^* and let $S(\alpha)$ and $S(\beta)$ be the associated series of differential operators. Then the composition of the two series $S(\alpha)$ and $S(\beta)$ is again a series $S(\alpha\beta)$, i.e.*

$$\forall g \in \mathcal{D}, S(\alpha) [S(\beta)[g]] = (S(\alpha)S(\beta))[g] = S(\alpha\beta)[g] \quad (2.3)$$

where $\alpha\beta = (\alpha \otimes \beta) \circ \Delta$.

Proof: The proof of this result is given in Theorem 24 of [Mur05]. \square

Given an algebra map $\alpha \in \text{Alg}(\mathcal{H}, \mathbb{R})$, we denote by $\beta = \log \alpha$ the map defining the corresponding vector field (see [Mur05] or [CHV05] for a formal definition and explicit formulas). Following [CMSS94], we will use the property that the value of $\alpha = \exp \beta$ for a forest $u \in \mathcal{F} \setminus \{e\}$ can be obtained as the solution at $\tau = 1$ of the differential equation

$$\begin{cases} \dot{\alpha}_\tau(u) &= (\alpha_\tau \beta)(u) \\ \alpha_0(u) &= 0, \end{cases} \quad (2.4)$$

with $\alpha_\tau(e) = 1$.

We end up this introductory section with a technical result which generalizes Lemma 3 in [CFM06] for coloured trees and a lemma giving an alternative expression of the co-product for trees of the form $t_1 \circ \dots \circ t_m$.

Lemma 2 *For any $(\omega_1, \dots, \omega_N) \in (\mathcal{H}^*)^N$, we have*

$$h \sum_{v=1}^N S(\omega_v) X(\bullet_v) = S(\omega'),$$

where ω' is defined by

$$\begin{aligned} \omega'(e) &= 0, \\ \forall u = t_1 \dots t_m \in \mathcal{F}, \quad \omega'(u) &= \sum_{i=1}^m \omega_{\mu(t_i)} \left(B^-(t_i) \prod_{j \neq i} t_j \right). \end{aligned}$$

Proof: Consider the expression (2.1) for the co-product. Now, let $\beta_v \in \mathcal{H}^*$ be such that $S(\beta_v) = hX(\bullet_v)$. Since $\beta_v(u) = 0$ unless $u = \bullet_v$, we have

$$\left(\sum_{v=1}^N \omega_v \beta_v\right)(t) = \sum_{v=1}^N (\omega_v \otimes \beta_v)(\Delta(t)) = \sum_{v=1}^N \omega_v(t) \beta_v(e) + \sum_{v=1}^N \sum_i \omega_v(u_i) \beta_v(s_i) = \omega_{\mu(t)}(B^-(t)).$$

For forests of $m \geq 2$ trees, we obtain:

$$\Delta(t_1 \dots t_m) = t_1 \dots t_m \otimes e + \sum_i u_i \otimes v_i,$$

where $v_i \in \mathcal{F}$ is a forest $v_i = s_1 \dots s_k$ of subtrees s_1, \dots, s_k of $1 \leq k \leq m$ trees amongst t_1, \dots, t_m and where u_i is the forest obtained when removing v_i from $t_1 \dots t_m$. As before, since $\beta_v(u) = 0$ unless $u = \bullet_v$, the only remaining terms are those for which $k = 1$, $v_i = \bullet_{\mu(t)}$ and $u_i = t_1 \dots t_{j-1} B^-(t_j) t_{j+1} \dots t_m$. \square

Lemma 3 For $t \in \mathcal{T}$ and $u, v, w \in \mathcal{F}$, define

$$\begin{aligned} (u \otimes t) \circ (v \otimes w) &= (uv \otimes t \circ w), \\ \bar{\Delta}(t) &= \Delta(t) - t \otimes e, \end{aligned}$$

then it holds that for arbitrary trees $t_1, \dots, t_m \in \mathcal{T}$, one can write

$$\begin{aligned} \Delta(t_1 \circ \dots \circ t_m) &= \delta(t_1, \dots, t_m) \otimes e \\ &+ \sum_{j=1}^{m-1} \Delta(t_1 \circ \dots \circ t_j) (\delta(t_{j+1} \circ \dots \circ t_m) \otimes e) + \bar{\Delta}(t_1) \circ \dots \circ \bar{\Delta}(t_m), \end{aligned} \quad (2.5)$$

$$\delta(t_1, \dots, t_m) = \sum_{k=1}^m (-1)^{k+1} \sum_{0=j_1 < \dots < j_{k+1}} \prod_{i=1}^k (t_{j_i+1} \circ \dots \circ t_{j_{i+1}}). \quad (2.6)$$

Proof: From the definitions of $\bar{\Delta}$ and of Δ , we easily get

$$\bar{\Delta}(\bullet_v) = e \otimes \bullet_v, \quad \bar{\Delta}(t \circ w) = \bar{\Delta}(t) \circ \Delta(w),$$

The identity (2.5) can then be proven from by induction on m . \square

3 Preservation of exact invariants

Given a differential equation of the form (1.1), we suppose that there exists a function $I(y)$ of y , which is kept invariant along any exact solution of the ODE corresponding to any individual vector field $f^{[v]}$, $v = 1, \dots, N$. We wish to derive conditions for a B-series integrator $B(\alpha)$ to preserve I , i.e.

$$I = I \circ B(\alpha) = S(\alpha)[I].$$

In terms of S -series, this reads

$$S(\alpha - id)[I] = 0,$$

where $id \in \mathcal{H}^*$ is such that $id(u) = 1$ for $u = e$ and $id(u) = 0$ for $u \neq e$. In other words, $\alpha - id$ should be an element of the annihilating left ideal $\mathcal{S}[I]$ of I : I being an invariant for each $f^{[v]}$, we have:

$$\forall v \in \{1, \dots, N\}, (\nabla I)^T f^{[v]} = 0, \quad (3.1)$$

that is to say, the Lie-derivative of I along any vector field $f^{[v]}$ is null. In terms of elementary differential operators, this is nothing else but saying that

$$X(\bullet_v)[I] = 0. \quad (3.2)$$

Since for any series of differential operators $S(\omega_1), S(\omega_2), \dots, S(\omega_N)$ acting respectively on $X(\bullet_1)[I], X(\bullet_2)[I], \dots, X(\bullet_N)[I]$ we have

$$\sum_{v=1}^N S(\omega_v)[hX(\bullet_v)[I]] = S(\omega')[I] = 0,$$

the inclusion $\{\delta \in \mathcal{H}^*; \exists \omega \in \mathcal{H}^*, \delta = \omega'\} \subset \mathcal{S}[I]$ follows.

We now look for conditions on δ such that $\delta = \omega'$. Writing this equality for trees gives

$$\forall t \in \mathcal{T}, \quad \delta(t) = \omega'(t) = \omega_{\mu(t)}(B^-(t))$$

which is equivalent to

$$\forall v \in \{1, \dots, N\}, \forall u \in \mathcal{F}, \quad \omega_v(u) = \delta(B_v^+(u)). \quad (3.3)$$

Given an arbitrary $\delta \in \mathcal{H}^*$, define the $\omega_v \in \mathcal{H}^*$ by (3.3), then $\delta = \omega'$ if and only if for all forests with at least two trees,

$$\begin{aligned} \delta(u) = \omega'(u) &= \sum_{i=1}^m \omega_{\mu(t_i)} \left(B^-(t_i) \prod_{j \neq i} t_j \right), \\ &\stackrel{\text{by (3.3)}}{=} \sum_{i=1}^m \delta \left(B_{\mu(t_i)}^+ (B^-(t_i) \prod_{j \neq i} t_j) \right). \end{aligned} \quad (3.4)$$

Using more conventional notations, the necessary and sufficient condition for the existence of $\omega \in \mathcal{H}^*$ such that $\delta = \omega'$ obtained above can be rewritten as

$$\delta(t_1 \cdots t_m) = \sum_{j=1}^m \delta \left(t_j \circ (t_1 \cdots t_{j-1} t_{j+1} \cdots t_m) \right), \quad (3.5)$$

where $t_j \circ (t_1 \cdots t_{j-1} t_{j+1} \cdots t_m)$ denotes the tree obtained by grafting the roots of $t_1, \dots, t_{j-1}, t_j, \dots, t_m$ to the root of t_j .

We have thus proven the following statement.

Lemma 4 Consider N vector fields $f^{[v]}$, $v = 1, \dots, N$, all having the same first integral I . Let $\delta \in \mathcal{H}^*$ be such that $\delta(e) = 0$. If condition (3.5) holds for all $m \geq 2$ and all $t_1, \dots, t_m \in \mathcal{T}$, then $S(\delta)[I] = 0$.

Next lemma is a consequence of standard arguments used to prove the independence of elementary differentials, see for instance [But87, HNW93].

Lemma 5 Given a forest $u = t_1 \dots t_m \in \mathcal{F}$ of order n , there exist polynomial maps $f^{[v]} : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $v = 1, \dots, N$ of degree less than $n - m + 1$ and $r : \mathbb{R}^n \rightarrow \mathbb{R}$ of degree m such that, for any $v \in \mathcal{F}$,

$$X(v)[r](0) \neq 0 \text{ iff } v = u. \quad (3.6)$$

Theorem 1 Let $\alpha \in \text{Alg}(\mathcal{H}, \mathbb{R})$. Then $S(\alpha)[I] = I$ for all $(N+1)$ -uplets $(f^{[1]}, f^{[2]}, \dots, f^{[N]}, I)$ of N vector fields $f^{[v]}$, $v = 1, \dots, N$, with first integral I , if and only if α satisfies the condition

$$\alpha(t_1) \cdots \alpha(t_m) = \sum_{j=1}^m \alpha(t_j \circ \prod_{i \neq j} t_i) \quad (3.7)$$

for all $m \geq 2$ and all $t_1, \dots, t_m \in \mathcal{T}$.

Proof: The proof follows step by step the proof of the corresponding result for $N = 1$. The only difference is that, in order to prove the necessity of the conditions, we need to consider the following differential system

$$\dot{y} = \sum_{v=1}^N f^{[v]}(y), \quad (3.8)$$

$$\dot{z} = - \sum_{v=1}^N (\nabla r(y))^T f^{[v]}(y), \quad (3.9)$$

where the $f^{[v]}$'s and r are chosen so as to satisfy condition (3.6) of Lemma 5 above, for a given $u \in \mathcal{F}$. It is clear that

$$I(y, z) = r(y) + z$$

is an invariant of (3.8-3.9) and of each individual system

$$\begin{aligned} \dot{y} &= f^{[v]}(y), \\ \dot{z} &= -(\nabla r(y))^T f^{[v]}(y). \end{aligned}$$

□

Remark 2 If $\beta = \log \alpha$ denotes the coefficients of the modified vector associated with the $S(\alpha)$ -series integrator, then an equivalent condition to (3.7) is:

$$0 = \sum_{j=1}^m \beta(t_j \circ \prod_{i \neq j} t_i) \quad (3.10)$$

It can be straightforwardly checked that the invariant $I(y, z) = g(y) + z$ constructed in the proof of Theorem 1 is a polynomial of degree m . This implies that conditions (3.7) for m trees are also necessary and sufficient for a B-series integrator to preserve polynomial first integrals up to degree m .

Theorem 2 *A B-series integrator that preserves all cubic polynomial invariants does in fact preserve polynomial invariants of any degree.*

Proof: This is a particular case of a more general result stated in Remark 24 of [Mur05]. Assume that condition (3.7) holds true for all $m \leq n$ with $n \geq 3$ and consider $p + q = n + 1$ trees $t_1, \dots, t_p, u_1, \dots, u_q$ in \mathcal{T} with $q \geq p \geq 2$. Denoting respectively by S_p and S_q the sum of the first p terms and of the last q terms of the right-hand side of (3.7), we can use equation (3.7) with $m = q + 1 \leq n$ and obtain

$$\begin{aligned} S_p &= \sum_i \alpha \left((t_i \circ \Pi_{j \neq i} t_j) \circ \Pi_k u_k \right), \\ &= - \sum_{i,k} \alpha \left(u_k \circ (t_i \circ \Pi_{j \neq i} t_j) \Pi_{l \neq k} u_l \right) + \sum_i \alpha (t_i \circ \Pi_{j \neq i} t_j) \Pi_k \alpha (u_k), \\ &= - \sum_{i,k} \alpha \left((u_k \circ \Pi_{l \neq k} u_l) \circ (t_i \circ \Pi_{j \neq i} t_j) \right) + \left(\Pi_i \alpha (t_i) \right) \left(\Pi_k \alpha (u_k) \right). \end{aligned}$$

A similar relation holds for S_q . Hence, $S_p + S_q - 2 \left(\Pi_i \alpha (t_i) \right) \left(\Pi_k \alpha (u_k) \right)$ can be written as

$$- \sum_{i,k} \left(\alpha \left((u_k \circ \Pi_{l \neq k} u_l) \circ (t_i \circ \Pi_{j \neq i} t_j) \right) + \alpha \left((t_i \circ \Pi_{j \neq i} t_j) \circ (u_k \circ \Pi_{l \neq k} u_l) \right) \right).$$

Now, using equation (3.7) with $m = 2$, we have

$$\begin{aligned} &\alpha \left((u_k \circ \Pi_{l \neq k} u_l) \circ (t_i \circ \Pi_{j \neq i} t_j) \right) + \alpha \left((t_i \circ \Pi_{j \neq i} t_j) \circ (u_k \circ \Pi_{l \neq k} u_l) \right) \\ &= \alpha (u_k \circ \Pi_{l \neq k} u_l) \alpha (t_i \circ \Pi_{j \neq i} t_j), \end{aligned}$$

so that, upon using (3.7) again with $m = p$ and $m = q$, we obtain

$$\sum_{i,k} \left(\alpha (u_k \circ \Pi_{l \neq k} u_l) \alpha (t_i \circ \Pi_{j \neq i} t_j) \right) = \left(\Pi_i \alpha (t_i) \right) \left(\Pi_k \alpha (u_k) \right). \quad (3.11)$$

As a consequence, relation (3.7) holds true for $m = n + 1$ and the stated result follows by induction. \square

At this stage, the question arises of whether there exist methods that satisfy conditions (3.7) for preservation of arbitrary first integrals. By assumption, the exact flow of each individual equation $\dot{y} = f^{[v]}(y)$, $v = 1, \dots, N$, preserves the first integral I . We then notice that numerical methods formed by composition of such flows also preserves I . By repeated application of the Baker-Campbell-Hausdorff formula, one can see that methods of this type can be formally interpreted as the exact flow of a vector field lying in the Lie-algebra generated by $f^{[1]}, \dots, f^{[N]}$. Conversely, any method that can be formally interpreted in that way preserves I . Next theorem states that they are the only ones.

Theorem 3 *A B-series integrator that preserves all cubic polynomial invariants can be formally interpreted as the exact flow of a vector field lying in the Lie-algebra generated by $f^{[1]}, \dots, f^{[N]}$.*

Proof: By Theorem 2, a B-series $B(\alpha)$ that preserves all cubic polynomials must necessarily satisfy condition (3.7), and then the required result follows from Remark 21 in [Mur05]. \square

4 Volume preserving integrators

In this section, we derive algebraic conditions for a B-series integrator to be volume-preserving. Since it is much easier to work with the divergence operator, we begin with deriving the conditions for a modified vector field to be divergence free.

4.1 Divergence-free B-series

Consider N divergence free vector fields $f^{[v]}$, $v = 1, \dots, N$. A B-series $B(\beta)$ with coefficients β satisfying $\beta(e) = 0$

$$\sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} \beta(t) F(t)$$

is divergence-free if and only if (using the linearity of the divergence operator)

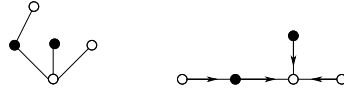
$$\sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} \beta(t) \operatorname{div}(F(t)) = 0. \quad (4.1)$$

The first problem we are thus confronted with is computing the divergence of each elementary differential vector field appearing in (4.1).

4.1.1 Aromatic trees

In order to conveniently represent $\operatorname{div}(F(t))$ for $t \in \mathcal{T}$, we introduce the following *aromatic trees*, which are certain connected oriented graphs with one cycle. Before defining them, we observe that coloured rooted trees can be interpreted as connected oriented graphs with coloured vertices as follows. Given $t \in \mathcal{T}$, let V be the set of vertices of t , then, the set $E \subset V \times V$ of arcs of the oriented graph identified with t is the set of pairs $(i, j) \in V \times V$ such that the vertex i is a child of the vertex j (i.e. j is the parent of i). Thus, the root of t is the only vertex $r \in V$ such that there is no $i \in V$ with $(r, i) \in E$. Furthermore, for each vertex $i \in V \setminus \{r\}$, there exist a unique sequence of vertices $j_1, \dots, j_m \in V$ ($m \geq 1$) such that $(i, j_1), (j_1, j_2), \dots, (j_{m-1}, j_m), (j_m, r) \in E$. Typically, a coloured rooted tree is graphically represented with the root at the bottom of the graph, and the children of each vertex positioned above it. When depicted as coloured oriented graphs, there is no need to draw the children of a vertex in any particular position with respect to their parent. Below, a coloured

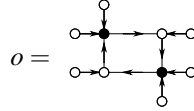
rooted tree is depicted in both the usual way and as a coloured oriented graph.



Similarly, a forest $t_1 \cdots t_m$ of coloured rooted trees can be identified with a coloured oriented graph whose connected components are identified with the rooted trees t_1, \dots, t_m .

Definition 3 An aromatic tree o is a coloured oriented graph with exactly one cycle, such that if all the arcs in the cycle are removed, then the resulting coloured oriented graph is identified with a forest $t_1 \cdots t_m$ of coloured rooted trees ($t_1, \dots, t_m \in \mathcal{T}$). If the arcs of o that form the cycle go from the root of t_i to the root of t_{i+1} ($i = 1, \dots, m-1$) and from the root of t_m to the root of t_1 then we write $o = (t_1 \cdots t_m)$. Note that $o = (t_1 \cdots t_m) = (t_i \cdots t_m t_1 \cdots t_{i-1})$ for all $i \in \{2, \dots, m\}$. The order $|o|$ of an aromatic tree $o = (t_1 \cdots t_m)$ is the number of its vertices, that is $|o| = |t_1| + \cdots + |t_m|$. The set of aromatic trees is denoted \mathcal{AT} and the set of n -th order aromatic trees \mathcal{AT}_n .

Example 3 For the aromatic tree



we have that $o = (t_1 t_2 t_1 t_2) = (t_2 t_1 t_2 t_1)$, where



Definition 4 For any aromatic tree $o = (t_1 \cdots t_m) \in \mathcal{AT}$, $C(o)$ is the unordered list of trees obtained from o by breaking any edge of the cycle. If we denote for $i = 1, \dots, m$, $s_i = t_i \circ t_{i+1} \circ \cdots \circ t_m \circ t_1 \circ \cdots \circ t_{i-1}$, where the grafting operation is meant to operate from right to left, then:

$$C(o) = \{s_1, \dots, s_m\}. \tag{4.2}$$

Now, let π_m be the circular permutation of $\{1, \dots, m\}$ and let θ be

$$\theta = \#\left\{l \in \{0, \dots, m-1\} : (t_{\pi_m^l(1)}, \dots, t_{\pi_m^l(m)}) = (t_1, \dots, t_m)\right\},$$

so that, for each i , there are θ copies of s_i in the list $C(o)$. Then the symmetry coefficient of o is defined as $\sigma(o) = \theta \prod_i \sigma(t_i)$.

Example 4 Consider again the aromatic tree o and the coloured rooted trees t_1, t_2 in Example 3. In that case, $\theta = 2$, and thus the symmetry coefficient is $\sigma(o) = 2\sigma(t_1)^2\sigma(t_2)^2 = 2$. As for the list of

coloured rooted trees in Definition 4, $C(o) = \{s_1, s_2, s_3, s_4\}$ where

$$\begin{aligned}
 s_1 &= \begin{array}{c} \circ \\ \downarrow \\ \bullet \\ \leftarrow \circ \quad \rightarrow \circ \\ \downarrow \quad \downarrow \\ \circ \quad \circ \end{array} = \begin{array}{c} \circ \quad \circ \\ \diagdown \quad \diagup \\ \bullet \\ \leftarrow \circ \quad \rightarrow \circ \\ \downarrow \\ \circ \end{array} = t_1 \circ t_2 \circ t_1 \circ t_2, \\
 s_2 &= \begin{array}{c} \circ \\ \downarrow \\ \bullet \\ \rightarrow \circ \quad \leftarrow \circ \\ \downarrow \quad \downarrow \\ \circ \quad \circ \end{array} = \begin{array}{c} \circ \quad \circ \\ \diagdown \quad \diagup \\ \bullet \\ \rightarrow \circ \quad \leftarrow \circ \\ \downarrow \\ \circ \end{array} = t_2 \circ t_1 \circ t_2 \circ t_1, \\
 s_3 &= \begin{array}{c} \circ \\ \downarrow \\ \bullet \\ \rightarrow \circ \quad \leftarrow \circ \\ \downarrow \quad \downarrow \\ \circ \quad \circ \end{array} = \begin{array}{c} \circ \quad \circ \\ \diagdown \quad \diagup \\ \bullet \\ \rightarrow \circ \quad \leftarrow \circ \\ \downarrow \\ \circ \end{array} = t_1 \circ t_2 \circ t_1 \circ t_2, \\
 s_4 &= \begin{array}{c} \circ \\ \downarrow \\ \bullet \\ \rightarrow \circ \quad \leftarrow \circ \\ \downarrow \quad \downarrow \\ \circ \quad \circ \end{array} = \begin{array}{c} \circ \quad \circ \\ \diagdown \quad \diagup \\ \bullet \\ \rightarrow \circ \quad \leftarrow \circ \\ \downarrow \\ \circ \end{array} = t_2 \circ t_1 \circ t_2 \circ t_1.
 \end{aligned}$$

For $t = [t_1, \dots, t_l]_v \in \mathcal{T}$, we shall use the notations of [AMSS97]

$$F^*(t) = \frac{\partial^{l+1} f^{[v]}}{\partial y^{l+1}} (F(t_1), \dots, F(t_l)),$$

so that

$$\frac{dF(t)}{\sigma(t)} = \frac{F^*(t)}{\sigma(t)} + \sum_{t_1 \circ t_2 \circ \dots \circ t_m = t} \frac{F^*(t_1)}{\sigma(t_1)} \frac{F^*(t_2)}{\sigma(t_2)} \dots \frac{F^*(t_m)}{\sigma(t_m)} \quad (4.3)$$

Definition 5 (Elementary divergence) The divergence $\text{div}(o)$ associated with an aromatic tree $o = (t_1 \dots t_m)$ is defined by:

$$\text{div}(o) = \text{Tr} \left(F^*(t_1) \dots F^*(t_m) \right). \quad (4.4)$$

It can be easily seen from the definition of $\text{div}(o)$ for $o \in \mathcal{A}\mathcal{T}$ that one has

$$\text{div} \left((t_1 \dots t_m) \right) = \text{div} \left((t_{\pi_m^l(1)} \dots t_{\pi_m^l(m)}) \right), \quad l \in \mathbb{N}. \quad (4.5)$$

This is the very reason for considering aromatic trees as cycles.

Remark 3 An alternative way of defining $\text{div}(o)$ for an aromatic tree o is as follows. Given $o \in \mathcal{AT}$, with $m = |o|$, represented as a coloured oriented graph with the set of indices $V = \{i_1, \dots, i_m\}$ as the set of vertices, coloured according to a map $\xi : V \rightarrow \{1, \dots, N\}$, and the set of arcs $E \subset V \times V$. Let for each $i \in V$ denote $g_i = f_{j_1, \dots, j_l}^{[v]i}$, where $v = \xi(i)$ (the colour of the vertex i), $\{j_1, \dots, j_l\} = \{j \in V : (j, i) \in E\}$, and $f_{j_1, \dots, j_l}^{[v]i}(y)$ is the partial derivative of the i th component of $f^{[v]}(y)$ with respect to the components y^{j_1}, \dots, y^{j_l} of $y \in \mathbb{R}^n$, then, it is not difficult to see that

$$\text{div}(o) = \sum_{i_1, \dots, i_m=1}^n g_{i_1} \cdots g_{i_m}.$$

4.1.2 Divergence-free conditions and first consequences

We are now in position to write in a convenient way the divergence of the modified vector field \tilde{f}_h given as a B-series $B(\beta)$. We first observe that, as $\text{div}(f^{[v]}) = 0$ for all $v = 1, \dots, N$, then $\text{Tr}(F^*(t)) = 0$ for all $t \in \mathcal{T}$. We thus have, by taking (4.3) into account,

$$\begin{aligned} \text{div}(B(\beta)) &= \sum_{t \in \mathcal{T}} \beta(t) \frac{h^{|t|}}{\sigma(t)} \text{div}(F(t)) = \sum_{t \in \mathcal{T}} \beta(t) h^{|t|} \text{Tr} \left(\frac{dF(t)}{\sigma(t)} \right) \\ &= \sum_{t \in \mathcal{T}} \beta(t) h^{|t|} \sum_{m \geq 2} \sum_{t_1 \circ \dots \circ t_m = t} \text{Tr} \left(\frac{F^*(t_1)}{\sigma(t_1)} \frac{F^*(t_2)}{\sigma(t_2)} \cdots \frac{F^*(t_m)}{\sigma(t_m)} \right) \\ &= \sum_{t \in \mathcal{T}} \beta(t) h^{|t|} \sum_{m \geq 2} \sum_{t_1 \circ \dots \circ t_m = t} \frac{\text{div}((t_1 \dots t_m))}{\sigma(t_1) \cdots \sigma(t_m)} \\ &= \sum_{n \geq 1} h^n \sum_{o \in \mathcal{AT}_n} \left(\sum_{t \in C(o)} \beta(t) \right) \frac{\text{div}(o)}{\sigma(o)}. \end{aligned}$$

Theorem 4 A modified field given by the B-series $B(\beta)$ is divergence-free up to order p if the following condition is satisfied:

$$\sum_{t \in C(o)} \beta(t) = 0 \text{ for all aromatic trees } o \in \mathcal{AT} \text{ with } |o| \leq p. \quad (4.6)$$

Theorem 5 Conditions (4.6) are necessary conditions for a vector-field to be divergence-free.

Proof: We will prove that, given $o \in \mathcal{AT}$ with $|o| = n$, there exist divergence free vector fields $f^{[v]} : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $v = 1, \dots, N$ and $y_0 \in \mathbb{R}^n$ such that $\text{div}(o)(y_0) = 1$ and for arbitrary $\hat{o} \in \mathcal{AT} \setminus \{o\}$, $\text{div}(\hat{o})(y_0) = 0$.

Given $o \in \mathcal{AT}_n$, we consider $y_0 = (0, \dots, 0)^T \in \mathbb{R}^n$, and $f^{[v]} : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $v = 1, \dots, N$, constructed as follows. Let o be represented as a coloured oriented graph with the set of vertices $V = \{1, \dots, n\}$, coloured according to a map $\xi : V \rightarrow \{1, \dots, N\}$, and the set of arcs $E \subset V \times V$. Then, for each $v = 1, \dots, N$ and each $i = 1, \dots, n$, the i th component $f^{[v]i}(y)$ of $f^{[v]}(y)$ ($y = (y^1, \dots, y^n)^T$)

is defined as

$$f^{[v]i}(y) = \begin{cases} \prod_{(j,i) \in E} y^j, & \text{if } \xi(i) = v, \\ 0 & \text{otherwise.} \end{cases}$$

Each such vector field $f^{[v]}$ is divergence free, as the main diagonal of its Jacobian matrix is identically null). The required result then follows, by taking Remark 3 into account, from the observation that, given $i, j_1, \dots, j_l \in V = \{1, \dots, n\}$, $f_{j_1, \dots, j_l}^{[v]i}(y_0) \neq 0$ if and only if $\{j_1, \dots, j_l\}$ (j_1, \dots, j_l being distinct) coincides with the set $\{j \in V : (j, i) \in E\}$. \square

Lemma 6 *The conditions for 2-cycles and 3-cycles are equivalent to the conditions for the preservation of all cubic polynomial invariants.*

Proof: For two-cycles and three-cycles, condition (4.6) can be written as

$$\forall (t_1, t_2) \in \mathcal{F}^2, b(t_1 \circ t_2) + b(t_2 \circ t_1) = 0, \quad (4.7)$$

and

$$\forall (t_1, t_2, t_3) \in \mathcal{F}^3, b(t_1 \circ t_2 \circ t_3) + b(t_2 \circ t_3 \circ t_1) + b(t_3 \circ t_1 \circ t_2) = 0 \quad (4.8)$$

respectively. Condition (4.7) is the symplecticity condition. As for condition (4.8), taking into account condition (4.7) and the induced relations

$$\begin{aligned} b(t_1 \circ t_2 \circ t_3) &= -b((t_2 \circ t_3) \circ t_1), \\ b(t_2 \circ t_3 \circ t_1) &= -b((t_3 \circ t_1) \circ t_2), \\ b(t_3 \circ t_1 \circ t_2) &= -b((t_1 \circ t_2) \circ t_3), \end{aligned}$$

it can be rewritten as

$$\forall (t_1, t_2, t_3) \in \mathcal{F}^3, b(t_1 \circ t_2 t_3) + b(t_2 \circ t_1 t_3) + b(t_3 \circ t_1 t_2) = 0,$$

which, together with (4.7), is the condition obtained in [CFM06] with $N = 1$ for modified fields to have solutions which preserve cubic invariants. \square

4.2 Volume-preserving B-series

The aim of this section is to rewrite the necessary and sufficient conditions (4.6) obtained for the modified field in terms of the coefficients of the B-series of the method itself.

A B-series that can be formally interpreted as the exact flow of a vector field lying in the Lie-algebra generated by $f^{[1]}, \dots, f^{[N]}$ is trivially volume-preserving (as the Lie bracket of divergence-free vector fields is also divergence-free). We can already state the following result on the non-existence of non trivial B-series methods preserving the volume:

Theorem 6 A volume-preserving B-series integrator can be formally interpreted as the exact flow of a vector field lying in the Lie-algebra generated by $f^{[1]}, \dots, f^{[N]}$.

Proof: This is a direct consequence of Lemma 6 and Theorem 3. \square

Definition 6 Consider an aromatic tree $o = (t_1 \dots t_m)$. If we remove $1 \leq k \leq m$ edges of the cycle o , we obtain a forest u with k trees. We denote by $C_k(o)$ the **list** of all possible forests obtained by removing any k edges from o .

Observe that $C_1(o)$ is denoted by $C(o)$ in Subsection 4.2.

Theorem 7 Consider a B-series integrator with coefficients α . $B(\alpha)$ preserves the volume up to order p if and only if the following conditions hold for all $1 \leq n \leq p$:

$$\forall o = (t_1 \dots t_m) \in \mathcal{AT}_n, \quad \sum_{k=1}^m (-1)^{k+1} \sum_{u \in C_k(o)} \alpha(u) = 0. \quad (4.9)$$

Proof: Assume that $\beta \in \mathcal{H}^*$ is such that $\beta(e) = 0$ and that, for arbitrary $t_1, \dots, t_m \in \mathcal{T}$,

$$\sum_{l=1}^m \beta(t_{\pi^l(1)} \circ \dots \circ t_{\pi^l(m)}) = 0.$$

According to Lemma 3, we have for $\alpha_\tau = e^{\tau\beta}$ as defined in (2.4)

$$\begin{aligned} \dot{\alpha}_\tau(t_1 \circ \dots \circ t_m) &= (\alpha_\tau \otimes \beta) \Delta(t_1 \circ \dots \circ t_m) \\ &= \sum_{j=1}^{m-1} \dot{\alpha}_\tau(t_1 \circ \dots \circ t_j) \alpha_\tau(\delta(t_{j+1} \circ \dots \circ t_m)) + (\alpha_\tau \otimes \beta)(\bar{\Delta}(t_1) \circ \dots \circ \bar{\Delta}(t_m)), \end{aligned} \quad (4.10)$$

where we have used the assumption that $\beta(e) = 0$. Thus

$$\begin{aligned} \sum_{l=1}^m \dot{\alpha}_\tau(t_{\pi^l(1)} \circ \dots \circ t_{\pi^l(m)}) &= \sum_{l=1}^m \left(\sum_{j=1}^{m-1} \dot{\alpha}_\tau(t_{\pi^l(1)} \circ \dots \circ t_{\pi^l(j)}) \alpha_\tau(\delta(t_{\pi^l(j+1)} \circ \dots \circ t_{\pi^l(m)})) \right) \\ &\quad + \sum_{l=1}^m (\alpha_\tau \otimes \beta)(\bar{\Delta}(t_{\pi^l(1)}) \circ \dots \circ \bar{\Delta}(t_{\pi^l(m)})). \end{aligned}$$

Since $\bar{\Delta}(t_{\pi^l(1)}) \circ \dots \circ \bar{\Delta}(t_{\pi^l(m)})$ is a linear combination of terms of the form

$$u \otimes \sum_{l=1}^m z_{\pi^l(1)} \circ \dots \circ z_{\pi^l(m)}, \quad (4.11)$$

where $u \in \mathcal{F}$ and $z_1, \dots, z_m \in \mathcal{T}$, the second term of previous sum vanishes and we get

$$\sum_{l=1}^m \dot{\alpha}_\tau(t_{\pi^l(1)} \circ \dots \circ t_{\pi^l(m)}) = \sum_{l=1}^m \sum_{j=1}^{m-1} \dot{\alpha}_\tau(t_{\pi^l(1)} \circ \dots \circ t_{\pi^l(j)}) \alpha_\tau(\delta(t_{\pi^l(j+1)} \circ \dots \circ t_{\pi^l(m)})),$$

or equivalently,

$$\sum_{l=1}^m \sum_{k=1}^m (-1)^{k+1} \sum_{0=j_1 < \dots < j_{k+1}} \dot{\alpha}_\tau(t_{\pi^l(j_1+1)} \circ \dots \circ t_{\pi^l(j_2)}) \prod_{i=2}^k \alpha_\tau(t_{\pi^l(j_{i+1})} \circ \dots \circ t_{\pi^l(j_i)}) = 0,$$

which after integration leads to the stated result. \square

4.2.1 Conditions for additive Runge-Kutta methods

In this section, we consider additive Runge-Kutta methods as described in [AMSS97]. Denoting the coefficients by $(a_{i,j}^{[1]}, b_i^{[1]}), \dots, (a_{i,j}^{[N]}, b_i^{[N]})$, we can define recursively

$$\Phi(\bullet_v) = (1, \dots, 1)^T \in \mathbb{R}^s, \quad (4.12)$$

$$\Phi([t_1 \dots t_m]_v) = \prod_{i=1}^m A^{[\mu(t_i)]} \Phi(t_i). \quad (4.13)$$

We then have $\alpha([t_1 \dots t_m]_v) = (b^{[v]})^T \Phi(t_i)$. Now, consider two trees t_1 and t_2 in \mathcal{T} . From the definition of Φ , we easily get

$$\Phi(t_1 \circ t_2) = \Phi(t_1) \cdot A^{[\mu(t_2)]} \Phi(t_2)$$

where \cdot denotes the componentwise product of vectors. More generally, for any m trees t_1, \dots, t_m of \mathcal{T} , it comes

$$\Phi(t_1 \circ t_2 \dots \circ t_m) = \Phi(t_1) A^{[\mu(t_2)]} \Phi(t_2) \dots A^{[\mu(t_m)]} \Phi(t_m),$$

where the products (matrix-vector product or componentwise vector product) operate from right to left. Denoting $X_i = \text{diag}(\Phi(t_i))$, we can thus write

$$\alpha(t_1 \circ t_2 \dots \circ t_m) = e^T B^{[\mu(t_1)]} X_1 A^{[\mu(t_2)]} X_2 \dots A^{[\mu(t_m)]} X_m e$$

and the coefficients $\alpha(u)$ for $u \in C_k((t_1 \dots t_m))$ all have the form

$$\prod_{i=1}^k (e^T B^{[\mu(t_{\pi^l(j_i)})]} X_{\pi^l(j_i)} \dots A^{[\mu(t_{\pi^l(j_{i+1-1})})]} X_{\pi^l(j_{i+1-1})} e),$$

where $l \in \{1, \dots, m\}$ and $1 = j_1 < j_2 < \dots < j_k = m + 1$.

Definition 7 An aromatic multi-index $\rho = (i_1^{[v_1]} \dots i_m^{[v_m]})$ is an oriented cycle where the vertices of the cycle are the coloured indices $i_1^{[v_1]}, i_2^{[v_2]}, \dots, i_m^{[v_m]}$. We denote by

$$C_1(\rho) = \left\{ (i_1^{[v_1]}, \dots, i_m^{[v_m]}), (i_2^{[v_2]}, \dots, i_m^{[v_m]}, i_1^{[v_1]}), \dots \right\}$$

the set of ordered multi-indices obtained by removing any edge of the cycle. If two edges of the cycle are removed, then we get pairs of ordered coloured multi-indices, and we denote by

$$C_2(\rho) = \left\{ \left((i_2^{[v_2]}, i_3^{[v_3]}), (i_4^{[v_4]}, \dots, i_m^{[v_m]}, i_1^{[v_1]}) \right), \dots \right\}$$

the set of such pairs; more generally, we denote by $C_k(\rho)$, $k = 1, \dots, m$ the set of k -uplets of ordered coloured multi-indices obtained by removing any k edges of the cycle.

Definition 8 Given an arbitrary ordered coloured multi-index $\bar{\omega} = i_1^{[v_1]} \dots i_l^{[v_l]}$, we define

$$\psi(i_1^{[v_1]} \dots i_l^{[v_l]}) := b_{i_1}^{[v_1]} a_{i_1 i_2}^{[v_2]} \dots a_{i_{l-1} i_l}^{[v_l]}.$$

and if $\mathbf{v} = (\bar{\omega}_1, \dots, \bar{\omega}_k)$ is a k -uplets of ordered multi-indices, then

$$\psi(\mathbf{v}) = \prod_{j=1}^k \psi(\bar{\omega}_j).$$

Then, the volume preserving condition for the m -cycle $\rho = (i_1^{[v_1]} \dots i_m^{[v_m]})$ reads

$$\sum_{k=1}^m (-1)^{k+1} \sum_{\mathbf{v} \in C_k(\rho)} \psi(\mathbf{v}) = 0, \quad \text{for each } (i_1^{[v_1]}, \dots, i_m^{[v_m]}) \in \{1, \dots, s\}^m. \quad (4.14)$$

It can be straightforwardly obtained from the conditions for the m -cycles $o = (t_1 \dots t_m)$ by letting t_1, \dots, t_m be arbitrary trees of colours respectively v_1, \dots, v_m . As a matter of fact, each matrix $X_l = \text{diag}(\Phi(t_l))$ then spans the whole set of diagonal matrices and the choice $(X_l)_{r,r} = \delta_{r,i_l}$ leads to (4.14).

Example 5 • For the coloured multi-index $\rho = (i^{[v_1]} j^{[v_2]})$, we obtain the conditions

$$b_i^{[v_1]} a_{ij}^{[v_2]} + b_j^{[v_2]} a_{ji}^{[v_1]} - b_i^{[v_1]} b_j^{[v_2]} = 0, \quad v_1, v_2 = 1, 2, \quad i, j = 1, \dots, s, \quad (4.15)$$

i.e. the symplecticity conditions for additive Runge-Kutta methods [AMSS97].

• For the cycle $\rho = (i^{[v_1]} j^{[v_2]} k^{[v_3]})$, we get,

$$\begin{aligned} b_i^{[v_1]} a_{ij}^{[v_2]} a_{jk}^{[v_3]} + b_j^{[v_2]} a_{jk}^{[v_3]} a_{ki}^{[v_1]} + b_k^{[v_3]} a_{ki}^{[v_1]} a_{ij}^{[v_2]} - b_i^{[v_1]} b_j^{[v_2]} a_{jk}^{[v_3]} - b_j^{[v_2]} b_k^{[v_3]} a_{ki}^{[v_1]} - b_k^{[v_3]} b_i^{[v_1]} a_{ij}^{[v_2]} \\ + b_i^{[v_1]} b_j^{[v_2]} b_k^{[v_3]} = 0, \quad v_1, v_2, v_3 = 1, \dots, 3, \quad i, j, k = 1, \dots, s. \end{aligned}$$

• Assume that we have one colour only. Taking $i = j = k$ in previous conditions gives

$$b_i(3a_{ii}^2 - 3b_i a_{ii} + b_i^2) = 0, \quad i = 1, \dots, s, \quad (4.16)$$

which has no other real solution than $b_1 = b_2 = \dots = b_s = 0$. This condition is by itself sufficient to prove that there exists no volume-preserving Runge-Kutta methods and as consequence, that no Runge-Kutta method can preserve polynomial invariants of degree greater than or equal to 3 (see [CIZ97, Zan98] and Theorem IV 3.3. of [HLW02]).

4.3 Systems with additional structure

We have so far obtained negative result about the existence of volume-preserving N -colour B-series integrators, apart from the trivial case of composition of exact flows of divergence-free vector fields (more precisely, apart from methods that can be formally interpreted as the exact flow of a vector field in the Lie algebra generated by the original vector fields in the splitting). In the present subsection, we consider three particular cases where the vector fields $f^{[v]}$ ($v = 1, \dots, N$) in have additional structure, such that volume-preserving B-series methods exists apart from the trivial case of composition of volume-preserving flows.

The first case we consider, is when each $f^{[v]}$ is actually a Hamiltonian vector field (hence divergence-free), so that, obviously, any symplectic B-series method applied to such decomposition of the original vector field is divergence-free (conservation of the symplectic form implies conservation of the volume form). We show algebraically that in that case, our volume-preservation conditions reduce to the symplecticity conditions in [AMSS97].

The second case we consider is a class of divergence-free systems split in two parts with a particular structure already considered in the literature (see [HLW02]). In such case, some symplectic methods (one-stage symplectic additive RK methods, and two-stage symplectic RK methods) turn out to be volume-preserving.

New volume-preserving methods for divergence-free systems split in three parts with a particular structure (generalization of the previous case) are considered as a third case. Similar results can also be obtained for further generalizations of divergence-free systems split in $N \geq 4$ parts, but we do not find it is worth doing it here.

4.3.1 Hamiltonian systems

For $f = \sum_{v=1}^N K^{-1} \nabla H^{[v]}$, where K is assumed to be an invertible skew-symmetric matrix, we have the following fundamental relation

$$\forall t \in \mathcal{T}, \quad (KF^*(t))^T = KF^*(t). \quad (4.17)$$

Now, let us consider the transposition operator τ defined on \mathcal{AT} as follows

$$\forall o = (t_1 \dots t_k) \in \mathcal{AT}, \tau(o) = (t_k t_{k-1} \dots t_1). \quad (4.18)$$

Due to relation (4.17), we have

$$\forall o = (t_1 \dots t_k) \in \mathcal{AT}, \quad \text{div}(o) = (-1)^k \text{div}(\tau(o)). \quad (4.19)$$

This can be easily seen by considering the following identity

$$\begin{aligned} \text{div}(o) &= \text{Tr}\left(F^*(t_1) \dots F^*(t_k)\right) = \text{Tr}\left(F^*(t_k)^T \dots F^*(t_1)^T\right) \\ &= (-1)^k \text{Tr}\left(KF^*(t_k)K^{-1} \dots KF^*(t_1)K^{-1}\right). \end{aligned}$$

Theorem 8 Suppose f is a sum of Hamiltonian parts (in possibly non-canonical form, i.e. K is just assumed to be an invertible skew-symmetric matrix) $f^{[V]} = K^{-1}\nabla H^{[V]}$. If the Hamiltonian conditions on the modified vector-field $B(b)$

$$\forall (u, v) \in \mathcal{T}^2, \quad b(u \circ v) + b(v \circ u) = 0, \quad (4.20)$$

or equivalently the symplecticity conditions on the B-series integrator $B(a)$

$$\forall (u, v) \in \mathcal{T}^2, \quad a(u \circ v) + a(v \circ u) = a(u)a(v), \quad (4.21)$$

are satisfied, then the flow \tilde{f}_h is divergence-free and the integrator volume-preserving.

Proof: Conditions for 2-cycles are satisfied by assumption. Now, consider a k -cycle $o = (t_1 \dots t_k)$, $k \in \mathbb{N}^*$, then $\text{div}(\tau(o)) = (-1)^k \text{div}(o)$. The two conditions corresponding to o and $\tau(o)$ can be merged into one:

$$\sum_{u \in C(o)} b(u) + (-1)^k \sum_{u \in C(\tau(o))} b(u) = 0. \quad (4.22)$$

Now, consider a tree $u \in C(o)$, for instance $u = t_1 \circ t_2 \circ \dots \circ t_k$. The tree $v = t_k \circ t_{k-1} \circ \dots \circ t_1$ belongs to $C(\tau(o))$ and we have $b(u) = (-1)^{k-1} b(v)$ since u and v belong to the same class of *free trees* and that the distance between their roots is $k-1$. Hence,

$$b(u) + (-1)^k b(v) = (1 + (-1)^{2k-1})b(u) = 0 \quad (4.23)$$

and condition (4.22) is satisfied. \square

4.3.2 Two-cycles systems

In this section, we consider the special situation of systems of the form

$$\begin{cases} \dot{p} = f(q) \\ \dot{q} = g(p) \end{cases}, \quad (4.24)$$

where f and g are smooth functions. In the framework of split systems, we can write them as

$$\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = f^{[1]}(q) + f^{[2]}(p), \quad (4.25)$$

with

$$f^{[1]}(q) = \begin{pmatrix} f(q) \\ 0 \end{pmatrix} \text{ and } f^{[2]}(p) = \begin{pmatrix} 0 \\ g(p) \end{pmatrix}.$$

Note that partitioned Runge-Kutta methods for systems of the form (4.24) can be interpreted as additive methods for (4.25). Now, consider B-series with two colours, with black vertices (corresponding to $f^{[1]}$) and white vertices (corresponding to $f^{[2]}$): due to the special form of (4.25), not all trees of

\mathcal{T} need to be considered: if $t = [t_1, \dots, t_m]_\bullet$, then $F(t)$ vanishes as soon as one of the t_i 's has a black root. The same obviously holds for trees with a white root so that only trees with vertices of *alternate* colours need to be considered. As for elementary divergences associated with aromatic trees, a lot also vanish: if $u = [v_1, \dots, v_m]_\bullet$ and $v = [u_1, \dots, u_n]_\circ$ have respectively a black and a white root, $F^*(u)$ and $F^*(v)$ have the following forms:

$$\begin{aligned} F^*(u) &= \frac{\partial^{m+1} f^{[1]}}{\partial(p,q)^{m+1}}(F(v_1), \dots, F(v_m)) = \begin{pmatrix} 0 & \eta(p,q) \\ 0 & 0 \end{pmatrix}, \\ F^*(v) &= \frac{\partial^{n+1} f^{[2]}}{\partial(p,q)^{m+1}}(F(u_1), \dots, F(u_n)) = \begin{pmatrix} 0 & 0 \\ \mu(p,q) & 0 \end{pmatrix}, \end{aligned}$$

with $\eta = \frac{\partial^{m+1} f}{\partial(p,q)^{m+1}}(F(v_1), \dots, F(v_m))$ and $\mu = \frac{\partial^{n+1} g}{\partial(p,q)^{m+1}}(F(u_1), \dots, F(u_n))$. Aromatic cycles composed of an odd number of trees are consequently irrelevant.

Lemma 7 *Let o be an aromatic tree of the form $o = (t_1 \cdots t_{2l+1})$ with $l \in \mathbb{N}$. Then the corresponding elementary divergence $\text{div}(o)$ is zero.*

Proof: Since o is composed of an odd number of trees, there exist two consecutive trees t_k and t_{k+1} in o (or possibly t_{2l+1} and t_1), with roots of the same colour, say for instance black. Then, we have

$$F^*(t_k)F^*(t_{k+1}) = \begin{pmatrix} 0 & \eta_k(p,q) \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \eta_{k+1}(p,q) \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},$$

and $\text{div}(o) = 0$. \square

Theorem 9 *A one-stage additive Runge-Kutta method formed of $(A^{[1]}, b^{[1]}) = (\theta_1, 1)$ and $(A^{[2]}, b^{[2]}) = (\theta_2, 1)$ is volume-preserving for systems of the form (4.24) if and only if $\theta_2 = 1 - \theta_1$, i.e. if and only if the method is symplectic.*

Proof: Consider an aromatic multi-index $\rho = (i_1^{[1]} \dots i_{2l}^{[2]})$ composed of $2l$ indices with colours in black/white order and let $v = (\varpi_1, \dots, \varpi_k) \in C_k(\rho)$. Since all quantities are scalar, the indices $i_1^{[1]}, \dots, i_{2l}^{[2]}$ take one and only value 1. Hence, if k_1 and k_2 denote the number of cuts before a respectively black and white root, we have

$$\psi(v) = \prod_{j=1}^k \psi(\varpi_j) = \theta_1^{l-k_1} \theta_2^{l-k_2},$$

and such a value of $\psi(v)$ can be obtained in

$$\binom{l}{k_1} \binom{l}{k_2} \tag{4.26}$$

different ways from ρ with $k = k_1 + k_2$ cuts. Hence, the condition for volume preservation becomes

$$\sum_{k=1}^{2l} (-1)^k \sum_{\substack{k_1+k_2=k, \\ 0 \leq k_1, k_2 \leq l}} \binom{l}{k_1} \binom{l}{k_2} \theta_1^{l-k_1} \theta_2^{l-k_2} = 0,$$

i.e.,

$$(\theta_1 - 1)(\theta_2 - 1) = \theta_1 \theta_2 \iff \theta_2 = 1 - \theta_1. \quad (4.27)$$

□

Theorem 10 *Two-stage symplectic Runge-Kutta methods are volume-preserving for separable systems of the form (4.24).*

Proof: Consider a 2-stage Runge-Kutta method with coefficient matrix $A \in \mathbb{R}^{2 \times 2}$ and $b \in \mathbb{R}^2$. One of the following two situations occur: either $\Phi(\bullet) = e$ and $\Phi(\mathcal{J}) = Ae := c$ are linearly independent or for all trees $t \in \mathcal{T}$, $\Phi(t)$ is co-linear to e . As matter of fact, if e and c are not linearly independent, being in a space of dimension 2 implies that $c = \lambda e$ for $\lambda \in \mathbb{R}$, and an easy induction then shows that $\Phi(t) = \lambda(t)e$, where $\lambda(t) \in \mathbb{R}$ for each $t \in \mathcal{A}\mathcal{T}$. The discussion in Subsection 4.2.1 shows that (4.9) holds for a given $m \geq 2$ and for all $o = (t_1 \cdots t_m) \in \mathcal{A}\mathcal{T}$, if it holds in the particular case where $t_1, \dots, t_m \in \{\bullet, \mathcal{J}\}$.

Let us write now the conditions for the modified vector field with coefficients $\beta = \log(\alpha)$ to be volume-preserving for the special situation of a cycle $o = (t_1 \dots t_{2m})$ with an even number of trees chosen in the set $\{\bullet, \mathcal{J}\}$:

$$\sum_{l=1}^{2m} \beta(t_{\pi^l(1)} \circ \dots \circ t_{\pi^l(2m)}) = 0. \quad (4.28)$$

We first recall that, owing to the symplecticity conditions, one has

$$\beta(t_{\pi^l(1)} \circ t_{\pi^l(2)} \circ \dots \circ t_{\pi^l(2m)}) = -\beta(t_{\pi^l(2m)} \circ t_{\pi^l(2m-1)} \circ \dots \circ t_{\pi^l(1)}).$$

One can easily check that the condition (4.28) is automatically satisfied provided that $t_1, \dots, t_{2m} \in \{\bullet, \mathcal{J}\}$.

Following the proof of Theorem 7 in the particular case where $t_1, \dots, t_{2m} \in \{\bullet, \mathcal{J}\}$, one observes that $\bar{\Delta}(t_{\pi^l(1)}) \circ \dots \circ \bar{\Delta}(t_{\pi^l(m)})$ is a linear combination of terms of the form (4.11), with $z_1, \dots, z_{2m} \in \{\bullet, \mathcal{J}\}$ (this is due to the fact that $\bar{\Delta}(\bullet) = e \otimes \bullet$ and $\bar{\Delta}(\mathcal{J}) = e \otimes \mathcal{J} + \bullet \otimes \bullet$). We thus have that, as (4.28) holds whenever $t_1, \dots, t_{2m} \in \{\bullet, \mathcal{J}\}$, then the volume preserving condition (4.9) holds for $o = (t_1, \dots, t_{2m})$ if $t_1, \dots, t_{2m} \in \{\bullet, \mathcal{J}\}$, which concludes the proof. □

4.3.3 Three-cycles systems

In this section, we consider the special situation of systems of the form

$$\begin{cases} \dot{p} &= \mathcal{F}(q) \\ \dot{q} &= \mathcal{G}(r) \\ \dot{r} &= \mathcal{H}(p) \end{cases}, \quad (4.29)$$

where F, G and H are smooth functions. In the framework of split systems, we can write them as

$$\begin{pmatrix} \dot{p} \\ \dot{q} \\ \dot{r} \end{pmatrix} = f^{[1]}(q) + f^{[2]}(r) + f^{[3]}(p),$$

with

$$f^{[1]}(q) = \begin{pmatrix} \mathcal{F}(q) \\ 0 \\ 0 \end{pmatrix}, f^{[2]}(r) = \begin{pmatrix} 0 \\ \mathcal{G}(r) \\ 0 \end{pmatrix} \text{ and } f^{[3]}(p) = \begin{pmatrix} 0 \\ 0 \\ \mathcal{H}(p) \end{pmatrix},$$

and consider 3-series, with black vertices (corresponding to $f^{[1]}$), white vertices (corresponding to $f^{[2]}$) and box vertices (corresponding to $f^{[3]}$). However, not all trees of \mathcal{AT} need to be considered: if $t = [t_1, \dots, t_m] \bullet$, then $F(t)$ vanishes as soon as one of the t_i 's has a black or a box root. The same obviously holds for trees with a white or a box root so that only trees with vertices of *alternate* colours in the order black/white/box need to be considered. As for elementary divergences associated with aromatic trees, a lot also vanish: if $u = [v_1, \dots, v_m] \bullet$, $v = [w_1, \dots, w_n] \circ$ and $w = [u_1, \dots, u_r] \square$ have respectively a black, a white and a box root, $F^*(u)$, $F^*(v)$ and $F^*(w)$ have the following forms:

$$\begin{aligned} F^*(u) &= \frac{\partial^{m+1} f^{[1]}}{\partial (p, q, r)^{m+1}} (F(v_1), \dots, F(v_m)) = \begin{pmatrix} 0 & \eta(p, q, r) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\ F^*(v) &= \frac{\partial^{n+1} f^{[2]}}{\partial (p, q, r)^{n+1}} (F(w_1), \dots, F(w_n)) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mu(p, q, r) \\ 0 & 0 & 0 \end{pmatrix}, \\ F^*(w) &= \frac{\partial^{r+1} f^{[3]}}{\partial (p, q, r)^{r+1}} (F(u_1), \dots, F(u_r)) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \xi(p, q, r) & 0 & 0 \end{pmatrix}, \end{aligned}$$

with $\eta = \frac{\partial^{m+1} \mathcal{F}}{\partial (p, q, r)^{m+1}} (F(v_1), \dots, F(v_m))$ and $\mu = \frac{\partial^{n+1} \mathcal{G}}{\partial (p, q, r)^{n+1}} (F(w_1), \dots, F(w_n))$ and $\xi = \frac{\partial^{r+1} \mathcal{H}}{\partial (p, q, r)^{r+1}} (F(u_1), \dots, F(u_r))$. Aromatic cycles composed of a number of trees which is not a multiple of 3 are consequently irrelevant.

Lemma 8 *Let o be an aromatic tree of the form $o = (t_1 \dots t_m)$. If there exists an index i in $\{1, \dots, m\}$ for which the three consecutive trees t_i, t_{i+1}, t_{i+2} (or t_{m-1}, t_m, t_1 if $i = m-1$ or t_m, t_1, t_2 if $i = m$) have roots that are not in the order black/white/box, then the corresponding elementary divergence $\text{div}(o)$ is zero. In particular, if $m = 3l + 1$ or $m = 3l + 2$, then $\text{div}(o)$ is zero.*

Proof: Consider three consecutive trees of the aromatic tree o , say for instance t_1 , t_2 and t_3 , and assume that they have roots which are not in the order black/white/box. For instance, let us suppose that t_1 has a black root. If t_2 also has a black root, then we have

$$F^*(t_1)F^*(t_2) = \begin{pmatrix} 0 & \eta_1(p, q, r) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & \eta_2(p, q, r) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

If t_2 has a box root, then we have similarly

$$F^*(t_1)F^*(t_2) = \begin{pmatrix} 0 & \eta_1(p, q, r) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \xi_2(p, q, r) & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

If t_2 has a white root, then it follows that

$$F^*(t_1)F^*(t_2) = \begin{pmatrix} 0 & \eta_1(p, q, r) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mu_2(p, q, r) \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & (\eta_1 \mu_2)(p, q, r) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

so that if t_3 has not a box root, then $F^*(t_1)F^*(t_2)F^*(t_3) = 0$ once again. In all cases where t_1, t_2 and t_3 have not their roots with colours in the order black/white/box, we thus get $\text{div}(o) = 0$. In particular, if $m = 3l + 1$ or $m = 3l + 2$, then there is necessarily such a sequence of three consecutive trees and $\text{div}(o) = 0$. \square

Theorem 11 *A one-stage additive Runge-Kutta method formed of $(A^{[1]}, b^{[1]}) = (\theta_1, 1)$, $(A^{[2]}, b^{[2]}) = (\theta_2, 1)$, and $(A^{[3]}, b^{[3]}) = (\theta_3, 1)$ is volume-preserving for systems of the form (4.29) if and only if*

$$(\theta_1 - 1)(\theta_2 - 1)(\theta_3 - 1) = \theta_1 \theta_2 \theta_3. \quad (4.30)$$

Proof: Consider an aromatic multi-index $\rho = (i_1^{[1]} \dots i_{3l}^{[3]})$ composed of $3l$ indices with colours in black/white/box order and let $v = (\varpi_1, \dots, \varpi_k) \in C_k(\rho)$. Since all quantities are scalar, the indices $i_1^{[1]}, \dots, i_{3l}^{[3]}$ take one and only value 1. Hence, if k_1, k_2 and k_3 denote the number of cuts before a respectively black, white and box root, we have

$$\psi(v) = \prod_{j=1}^k \psi(\varpi_j) = \theta_1^{l-k_1} \theta_2^{l-k_2} \theta_3^{l-k_3},$$

and such a value of $\psi(v)$ can be obtained in

$$\binom{l}{k_1} \binom{l}{k_2} \binom{l}{k_3} \quad (4.31)$$

different ways from ρ with $k = k_1 + k_2 + k_3$ cuts. Hence, the condition for volume preservation becomes

$$\sum_{k=1}^{3l} (-1)^k \sum_{\substack{k_1+k_2+k_3=k, \\ 0 \leq k_1, k_2, k_3 \leq l}} \binom{l}{k_1} \binom{l}{k_2} \binom{l}{k_3} \theta_1^{l-k_1} \theta_2^{l-k_2} \theta_3^{l-k_3} = 0,$$

i.e., if (4.30) holds. \square

Example 6 *The method corresponding to $(\theta_1, \theta_2, \theta_3) = (0, 1/2, 1)$ (i.e. Explicit Euler / Midpoint / Implicit Euler) can be written for systems of the form (4.29) as*

$$\begin{aligned} p_1 &= p_0 + h\mathcal{F}\left(\frac{q_1 + q_0}{2}\right) \\ q_1 &= q_0 + h\mathcal{G}(r_1) \\ r_1 &= r_0 + h\mathcal{H}(p_0) \end{aligned}$$

and is thus explicit, and it is equivalent to the composition of exact flows for $f^{[1]}$, $f^{[2]}$ and $f^{[3]}$. As additional example, consider $(\theta_1, \theta_2, \theta_3) = (1/3, 4/3, 1/3)$, so that the corresponding additive RK method reads

$$\begin{aligned} P &= p_0 + \frac{h}{3}\mathcal{F}(Q) & p_1 &= p_0 + h\mathcal{F}(Q) \\ Q &= q_0 + \frac{4h}{3}\mathcal{G}(R) & q_1 &= q_0 + h\mathcal{G}(R) \\ R &= r_0 + \frac{h}{3}\mathcal{H}(P) & r_1 &= p_0 + h\mathcal{H}(P) \end{aligned}$$

and is not explicit.

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