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Preserving first integrals and volume forms of additively split systems

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This work is concerned with the preservation of invariants and volume forms by numerical methods which can be expanded into B-series. The situation we consider here is that of a split vector field $f = f^{[1]} + \cdots + f^{[N]}$, where each $f^{[\nu]}$ 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 nonexistence results. For a more restrictive class of problems, where the system is partitioned into several components, we nevertheless obtain simplified conditions and show that they can be solved.

Keywords: polynomial invariants; volume form; split systems; B-series; S-series.

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 integrals[1] and as a consequence that no volume-preserving B-series method exists apart from the composition of exact flows (see Theorem 4.10 of Section 4.2). This result generalizes to split vector fields, a known result of Feng & Shang (1995). Let us note that a similar result, using rather different techniques of proof, has been derived independently by Iserles *et al.* (2006b). 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 (RK) method (see Section 4.2.1).

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

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[1] The fact that no RK method can preserve polynomial invariants of degree less than or equal to 3 was first shown by Calvo *et al.* (1997) and the extension of this result to arbitrary degree was considered in Zanna (1998) and Iserles & Zanna (2000). Here, we extend this result to arbitrary B-series for split vector fields.

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 and three functions. The results obtained for two functions corroborate already known ones (see Hairer *et al.*, 2002, Theorem 3.4) and results for more than three functions (and their straightforward generalization to more functions) appear to be completely new. It is interesting to note that the general idea used here to obtain numerical methods also has some similarities with the technique considered by Iserles *et al.* (2006a) for polynomial vector fields.

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

$$\dot{y}(x) = \sum_{\nu=1}^{N} f^{[\nu]}(y) \tag{1.1}$$

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

An NB-series $\mathrm{NB}(a)$ is a formal expression of the form

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

where the index set $\mathscr{T}$ is the set of N-coloured rooted trees, $|\cdot|$, σ and F are real functions defined on $\mathscr{T}$ and a is a function defined on $\mathscr{T}$ as well which characterizes the NB-series itself. These series have been introduced in Araújo *et al.* (1997) in full details for the purpose of studying symplectic additive RK methods. Note that this definition coincides with the standard definition of B-series as given in Hairer *et al.* (2002) 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 Chartier *et al.* (2006), S-series arises 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, an S-series is a series of the form

$$\begin{aligned} S(\alpha)[g] = {} & \alpha(e)g + h\alpha(\bullet)g_y f^{[1]} + h\alpha(\circ)g_y f^{[2]} \\ & + h^2\left(\frac{\alpha(\bullet\,\bullet)}{2} g_{yy}(f^{[1]}, f^{[1]}) + \alpha(\bullet\,\circ) g_{yy}(f^{[1]}, f^{[2]}) + \frac{\alpha(\circ\,\circ)}{2} g_{yy}(f^{[2]}, f^{[2]})\right) \\ & + h^2\big(\alpha\big(\substack{\bullet\\ \mid \\ \bullet}\big) g_y f_y^{[1]} f^{[1]} + \alpha\big(\substack{\circ\\ \mid \\ \bullet}\big) g_y f_y^{[1]} f^{[2]} + \alpha\big(\substack{\bullet\\ \mid \\ \circ}\big) g_y f_y^{[2]} f^{[1]} + \alpha\big(\substack{\circ\\ \mid \\ \circ}\big) g_y f_y^{[2]} f^{[2]}\big) + \cdots. \end{aligned}$$

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

$$\forall\, \nu = 1, \ldots, N, \quad \forall\, y \in \mathbb{R}^n, \quad (\nabla I(y))^{\mathrm{T}} f^{[\nu]}(y) = 0, \tag{1.4}$$

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

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

and it can be shown (Murua, 1999) that

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

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

Assuming now that we have, instead of (1.4),

$$\forall\, \nu = 1, \ldots, N, \quad \forall\, y \in \mathbb{R}^n, \quad \operatorname{div} f^{[\nu]}(y) = 0,$$

preserving the volume for an integrator whose modified vector field is $\tilde{f}_h(y) = \frac{1}{h} B(\beta)(y)$ amounts to satisfying the condition

$$\forall\, y \in \mathbb{R}^n, \quad \operatorname{div}(\tilde{f}_h(y)) = 0.$$

Using the 'linearity' of the divergence operator and a convenient matrix representation of the differential forms $\mathrm{d}F(t)$ for a tree t, we obtain algebraic conditions in terms of 'aromatic' trees, defined as oriented trees with exactly one cycle. Anticipating on the computations of Section 4.2, consider, for instance, the term $\operatorname{div}(F([\bullet\,\circ]_1))$ as appearing in $\operatorname{div}(\tilde{f}_h)$. We have

$$\begin{aligned}
\operatorname{div}(F([\bullet\,\circ]_1)) &= \operatorname{Tr}\frac{\partial}{\partial y}(f^{[1]}_{yy}(f^{[1]}, f^{[2]})) \\
&= \operatorname{Tr}(f^{[1]}_{yyy}(f^{[1]}, f^{[2]}, \cdot)) + \operatorname{Tr}(f^{[1]}_{yy}(f^{[1]}_{y}\cdot, f^{[2]})) + \operatorname{Tr}(f^{[1]}_{yy}(f^{[1]}, f^{[2]}_{y}\cdot)) \\
&:= \operatorname{Tr}(F^*([\bullet\,\circ]_1)) + \operatorname{Tr}(F^*([\bullet]_1)F^*(\circ)) + \operatorname{Tr}(F^*([\circ]_1)F^*(\bullet)) \\
&:= \operatorname{div}(o_1) + \operatorname{div}(o_2) + \operatorname{div}(o_3),
\end{aligned}$$

where $F^*(t)$ denotes the matrix obtained by differentiating $F(t)$ 'at the root of t' and $o_1 = (t)$, $o_2 = ([\bullet]_1\,\circ)$ and $o_3 = ([\circ]_1\,\bullet)$ are aromatic trees composed, respectively, of one, two and two trees. Note that owing to the properties of the trace operator, $\operatorname{div}([\bullet]_1\,\circ) = \operatorname{div}(\circ\,[\bullet]_1)$, so that there is no reason to distinguish $([\bullet]_1\,\circ)$ from $(\circ\,[\bullet]_1)$: this general property allows us to consider such expressions as trees with one cycle. It will turn out that the algebraic conditions for volume preservation can be expressed solely in terms of aromatic trees.

2. Basic tools

In this 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 Chartier *et al.* (2006), we shall focus mainly on the differences with the one-colour situation.

2.1 *The algebra of trees*

DEFINITION 2.1 (Rooted trees, forests) The set of (rooted) trees $\mathscr{T}$ and forests $\mathscr{F}$ are defined recursively by the following:

1. the forest e is the empty forest;
2. if $t_1, \ldots, t_n$ are n trees of $\mathscr{T}$, the forest $u = t_1 \cdots t_n$ is the commutative juxtaposition of $t_1, \ldots, t_n$;
3. if u is a forest of $\mathscr{F}$, then $t = [u]_\nu$, where $\nu \in \{1, \ldots, N\}$, is a tree of $\mathscr{T}$ with root of colour ν.

The order of a tree is its number of vertices and is denoted by $|t|$. The order $|u|$ of a forest $u = t_1 \cdots t_n$ is the sum of the $|t_i|$ values. If $u = t_1^{r_1} \cdots t_n^{r_n}$, where $t_1, \ldots, t_n$ are pairwise distinct and are repeated,

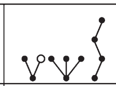
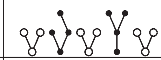
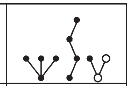
Forest u				
Order $\|u\|$	4	11	17	11
Symmetry $\sigma(u)$	$2!$	$1!3!1!$	$3!(2!)^3 2!$	$3!1!1!$

FIG. 1. A few forests with their orders and symmetry coefficients.

respectively, $r_1, \ldots, r_n$ times, then the symmetry σ of u is

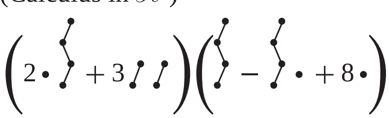
$$\sigma(u) = r_1! \cdots r_n! (\sigma(t_1))^{r_1} \cdots (\sigma(t_n))^{r_n}.$$

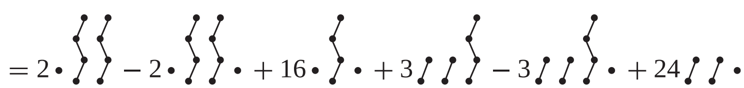
By convention, $\sigma(e) = 1$. The symmetry $\sigma(t)$ of a tree $t = [u]_\nu$ is the symmetry of u. The set of linear combinations of forests in $\mathscr{F}$ can be naturally endowed with an algebra structure $\mathscr{H}$, and the tensor product of $\mathscr{H}$ with itself can be defined just as in Chartier *et al.* (2006).

DEFINITION 2.2 The algebra of forests $\mathscr{H}$ is defined as follows:

- $\forall (u, v) \in \mathscr{F}^2, \forall (\lambda, \mu) \in \mathbb{R}^2, \lambda u + \mu v \in \mathscr{H}$,
- $\forall (u, v) \in \mathscr{F}^2, uv \in \mathscr{H}$ (note that $uv = vu$),
- $\forall u \in \mathscr{F}, ue = eu = u$.

EXAMPLE 2.3 (Calculus in $\mathscr{H}$)





DEFINITION 2.4 The tensor product of $\mathscr{H}$ with itself is the set of elements of the form $u \otimes v$ such that for all $(u, v, w, x) \in \mathscr{H}^4$ and all $(\lambda, \mu) \in \mathbb{R}^2$,

$$(\lambda u + \mu v) \otimes w = \lambda(u \otimes w) + \mu(v \otimes w),$$

$$w \otimes (\lambda u + \mu v) = \lambda(w \otimes u) + \mu(w \otimes v),$$

$$(u \otimes v)(w \otimes x) = (uw \otimes vx).$$

We will further denote by $\mathrm{Alg}(\mathscr{H}, \mathbb{R})$ the space of algebra morphisms from $\mathscr{H}$ to $\mathbb{R}$, i.e. maps from $\mathscr{H}$ to $\mathbb{R}$ such that

$$\forall u = t_1 \cdots t_m \in \mathscr{F}, \quad \alpha(u) = \alpha(t_1) \cdots \alpha(t_m),$$

and by $\mathscr{H}^*$ the space of linear forms on $\mathscr{H}$. Eventually, the co-product has to take into account the possibility of trees with different colours. Hence, the operator B^+ becomes B^+_ν as defined below:

$$B^+_\nu : \quad \mathscr{F} \quad \to \quad \mathscr{T},$$
$$u = t_1 \cdots t_n \mapsto [t_1 \cdots t_n]_\nu.$$

EXAMPLE 2.5

$$B_1^+(\bullet\circ) = [\bullet\circ]_1 = \quad , \quad B_2^+(\bullet\bullet) = [\bullet\bullet]_2 = \quad , \quad B^-(\quad) = \bullet\bullet\bullet, \quad B^-\Big(\quad\Big) = \quad .$$

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

DEFINITION 2.6 (Co-product) The co-product Δ is a 'linear' map from $\mathscr{H}$ to $\mathscr{H} \otimes \mathscr{H}$ defined recursively by the following:

1. $\Delta(e) = e \otimes e$,
2. $\forall t \in \mathscr{T}$, $\Delta(t) = t \otimes e + (\mathrm{id}_{\mathscr{H}} \otimes B^+_{\mu(t)}) \circ \Delta \circ B^-(t)$,
3. $\forall u = t_1 \cdots t_n \in \mathscr{F}$, $\Delta(u) = \Delta(t_1) \cdots \Delta(t_n)$.

EXAMPLE 2.7

$$\begin{aligned}
\Delta(\quad) &= \quad \otimes e + (id_{\mathscr{H}} \otimes B_2^+)\Delta(\bullet\circ) \\
&= \quad \otimes e + (id_{\mathscr{H}} \otimes B_2^+)\Delta(\bullet)\Delta(\circ) \\
&= \quad \otimes e + (id_{\mathscr{H}} \otimes B_2^+)(\bullet \otimes e + e \otimes \bullet)(\circ \otimes e + e \otimes \circ) \\
&= \quad \otimes e + (id_{\mathscr{H}} \otimes B_2^+)(\bullet\circ \otimes e + \bullet \otimes \circ + \circ \otimes \bullet + e \otimes \bullet\circ) \\
&= \quad \otimes e + \bullet\circ \otimes \circ + \bullet \otimes \quad + \circ \otimes \quad + e \otimes \quad .
\end{aligned}$$

REMARK 2.8 The co-product of a tree can also be written as (see Connes & Kreimer, 1998, for instance)

$$\Delta(t) = t \otimes e + \sum_i u_i \otimes s_i, \tag{2.1}$$

where $s_i \in \mathscr{T}$ 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 $t \in \mathscr{T}$, the 'elementary differential' $F^{[\nu]}(t)$ is a mapping from $\mathbb{R}^n$ to $\mathbb{R}^n$ defined recursively by

$$F(\bullet_\nu)(y) = f^{[\nu]}(y), \quad F([t_1 \cdots t_n]_\nu)(y) = \frac{\partial^n f^{[\nu]}}{\partial y^n}(y)(F(t_1)(y), \ldots, F(t_n)(y)),$$

where $\bullet_\nu = [e]_\nu$.

EXAMPLE 2.9

$$F(\quad) = f_y^{[1]} f^{[2]}, \quad F(\quad) = f_{yy}^{[2]}(f^{[1]}, f^{[2]}), \quad F(\quad) = f_y^{[1]} f_y^{[2]} f^{[1]}.$$

We can now define formally a coloured B-series as follows.

DEFINITION 2.10 (B-Series) Let $a\colon \mathscr{T} \to \mathbb{R}$. The B-series $B(a)$ is the formal series

$$B(a)(y) = a(e)y + \sum_{t\in\mathscr{T}} \frac{h^{|t|}}{\sigma(t)} a(t)F(t)(y).$$

EXAMPLE 2.11 The B-series corresponding to the implicit/explicit Euler method is of the form

$$\begin{aligned} y_1 &= y_0 + h(f^{[1]}(y_1) + f^{[2]}(y_0)) \\ &= y_0 + hF(\bullet)(y_0) + hF(\circ)(y_0) + h^2F(\;)(y_0) + h^2F(\;)(y_0) + \mathscr{O}(h^3). \end{aligned}$$

Differential operators associated to a forest and S-series are exactly the same as for the one-colour situation (Chartier *et al.*, 2006).

DEFINITION 2.12 (Differential operator associated to a forest (Merson, 1957)) Consider a forest $u = t_1 \cdots t_k$ of $\mathscr{F}$. The differential operator $X(u)$ associated to u is the map operating on smooth functions $\mathscr{D} = C^\infty(\mathbb{R}^n; \mathbb{R}^m)$, defined as

$$\begin{aligned} X(u)\colon \mathscr{D} &\to \mathscr{D}, \\ g &\mapsto X(u)[g] = g^{(n)}(F(t_1), \ldots, F(t_k)). \end{aligned}$$

EXAMPLE 2.13 For $g \in \mathscr{D}$, one has

$$X(e)[g] = g, \quad X(\bullet_\nu)[g] = g_y f^{[\nu]},$$

$$X(\;)[g] = g_y f_y^{[1]} f^{[2]}, \quad X(\; \bullet \circ) = g_{yyy}(f_y^{[2]} f^{[1]}, f^{[1]}, f^{[2]}).$$

More generally, the relations

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

hold true.

DEFINITION 2.14 (Series of differential operators) Let $\alpha\colon \mathscr{F} \to \mathbb{R}$. The S-series $S(\alpha)$ is the formal series

$$S(\alpha)[g] = \sum_{u\in\mathscr{F}} \frac{h^{|u|}}{\sigma(u)} \alpha(u)X(u)[g].$$

Now, considering the action of a map $g \in \mathscr{D}$ on a B-series $B(a)$, the following formula can be easily obtained (see, for instance, Murua (1999) for a proof):

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

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

LEMMA 2.15 (Composition of S-series) Let α and β be in $\mathscr{H}^*$ 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.

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

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

Proof. The proof of this result is given in Theorem 24 of Murua (2006). □

Given an algebra map $\alpha \in \mathrm{Alg}(\mathscr{H}, \mathbb{R})$, we denote by $\beta = \log \alpha$ the map defining the corresponding vector field (see Murua (2006) or Chartier *et al.* (2005) for a formal definition and explicit formulas). Following Calvo *et al.* (1994), we will use the property that the value of $\alpha = \exp \beta$ for a forest $u \in \mathscr{F} \backslash \{e\}$ can be obtained as the solution at $\tau = 1$ of the differential equation

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

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

We end up this introductory section with a technical result which generalizes Lemma 3 in Chartier *et al.* (2006) for coloured trees and a lemma giving an alternative expression of the co-product for trees of the form $t_1 \circ \cdots \circ t_m$, where $\circ$ is the so-called Butcher product[2] and is meant to operate from right to left in expressions like $t_1 \circ t_2 \circ \cdots \circ t_m$.

LEMMA 2.16 For any $(\omega_1, \ldots, \omega_N) \in (\mathscr{H}^*)^N$, we have

$$h \sum_{\nu=1}^{N} S(\omega_\nu) X(\bullet_\nu) = S(\omega'),$$

where ω' is defined by

$$\omega'(e) = 0,$$

$$\forall\, u = t_1 \cdots t_m \in \mathscr{F}, \quad \omega'(u) = \sum_{i=1}^{m} \omega_{\mu(t_i)} \left(B^-(t_i) \prod_{j \neq i} t_j \right).$$

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

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

For forests of $m \geqslant 2$ trees, we obtain

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

[2] If t_1 and t_2 are two trees, $t_1 \circ t_2$ is the tree obtained by grafting the root of t_2 onto the root of t_1.

where $v_i \in \mathscr{F}$ is a forest, $v_i = s_1 \cdots s_k$, of subtrees $s_1, \ldots, s_k$ of $1 \leqslant k \leqslant m$ trees among $t_1, \ldots, t_m$ and u_i is the forest obtained when removing v_i from $t_1 \cdots t_m$. As before, since $\beta_\nu(u) = 0$ unless $u = \bullet_\nu$, the only remaining terms are those for which $k = 1$, $v_i = \bullet_{\mu(t)}$ and $u_i = t_1 \cdots t_{j-1} B^-(t_j) t_{j+1} \cdots t_m$. □

LEMMA 2.17 For $t \in \mathscr{T}$ and $u, v, w \in \mathscr{F}$, define

$$(u \otimes t) \circ (v \otimes w) = (uv \otimes t \circ w),$$

$$\bar{\Delta}(t) = \Delta(t) - t \otimes e,$$

then for arbitrary trees $t_1, \ldots, t_m \in \mathscr{T}$ one can write

$$\Delta(t_1 \circ \cdots \circ t_m) = \delta(t_1, \ldots, t_m) \otimes e + \sum_{j=1}^{m-1} \Delta(t_1 \circ \cdots \circ t_j)(\delta(t_{j+1} \circ \cdots \circ t_m) \otimes e) + \bar{\Delta}(t_1) \circ \cdots \circ \bar{\Delta}(t_m), \tag{2.5}$$

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

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

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

The identity (2.5) can then be proved by induction on m. □

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 ordinary differential equation corresponding to any individual vector field $f^{[\nu]}$, $\nu = 1, \ldots, N$. 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 $id \in \mathscr{H}^*$ 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 $\mathscr{I}[I]$ of I. I being an invariant for each $f^{[\nu]}$, we have

$$\forall \nu \in \{1, \ldots, N\}, \quad (\nabla I)^{\mathrm{T}} f^{[\nu]} = 0, \tag{3.1}$$

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

$$X(\bullet_\nu)[I] = 0. \tag{3.2}$$

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

$$\sum_{\nu=1}^{N} S(\omega_\nu)[hX(\bullet_\nu)[I]] = S(\omega')[I] = 0,$$

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

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

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

which is equivalent to

$$\forall\, \nu \in \{1, \ldots, N\}, \;\; \forall\, u \in \mathscr{F}, \quad \omega_\nu(u) = \delta(B_\nu^+(u)). \tag{3.3}$$

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

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

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

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

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 $t_1, \ldots, t_{j-1}, t_j, \ldots, t_m$ onto the root of t_j.

We have thus proved the following statement.

LEMMA 3.1 Consider N vector fields $f^{[\nu]}$, $\nu = 1, \ldots, N$, all having the same first integral I. Let $\delta \in \mathscr{H}^*$ be such that $\delta(e) = 0$. If condition (3.5) holds for all $m \geqslant 2$ and all $t_1, \ldots, t_m \in \mathscr{T}$, then $S(\delta)[I] = 0$.

The next lemma is a consequence of standard arguments used to prove the independence of elementary differentials (see, for instance, Butcher, 1987; Hairer *et al.*, 1993).

LEMMA 3.2 Given a forest $u = t_1 \cdots t_m \in \mathscr{F}$ of order n, there exist polynomial maps $f^{[\nu]}: \mathbb{R}^n \to \mathbb{R}^n$, $\nu = 1, \ldots, N$, of degree less than $n - m + 1$ and $r: \mathbb{R}^n \to \mathbb{R}$ of degree m such that, for any $v \in \mathscr{F}$,

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

THEOREM 3.3 Let $\alpha \in \mathrm{Alg}(\mathscr{H}, \mathbb{R})$. Then, $S(\alpha)[I] = I$ for all $(N+1)$-tuplets $(f^{[1]}, f^{[2]}, \ldots, f^{[N]}, I)$ of N vector fields $f^{[\nu]}$, $\nu = 1, \ldots, N$, with first integral I if, and only if, α satisfies the condition

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

for all $m \geqslant 2$ and all $t_1, \ldots, t_m \in \mathscr{T}$.

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:

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

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

where the $f^{[\nu]}$ values and r are chosen so as to satisfy condition (3.6) of Lemma 3.2 above, for a given $u \in \mathscr{F}$. It is clear that

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

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

$$\dot{y} = f^{[\nu]}(y),$$
$$\dot{z} = -(\nabla r(y))^{\mathrm{T}} f^{[\nu]}(y).$$

□

REMARK 3.4 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

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

It can be straightforwardly checked that the invariant $I(y, z) = g(y) + z$ constructed in the proof of Theorem 3.3 is a polynomial of degree m. This implies that condition (3.7) for m trees is also necessary and sufficient for a B-series integrator to preserve polynomial first integrals up to degree m.

THEOREM 3.5 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 Murua (2006). Assume that Condition (3.7) holds true for all $m \leqslant n$ with $n \geqslant 3$ and consider $p + q = n + 1$ trees, $t_1, \ldots, t_p$,

$u_1, \dots, u_q$, in $\mathscr{T}$ with $q \geqslant p \geqslant 2$. 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 (3.7) with $m = q+1 \leqslant n$ and obtain

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

A similar relation holds for S_q. Hence, $S_p + S_q - 2\big(\prod_i \alpha(t_i)\big)\big(\prod_k \alpha(u_k)\big)$ can be written as

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

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

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

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

$$\sum_{i,k}\left(\alpha\left(u_k \circ \prod_{l\neq k} u_l\right) \alpha\left(t_i \circ \prod_{j\neq i} t_j\right)\right) = \left(\prod_i \alpha(t_i)\right)\left(\prod_k \alpha(u_k)\right). \tag{3.11}$$

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

At this stage, the question arises as to whether there exist methods that satisfy condition (3.7) for preservation of arbitrary first integrals. By assumption, the exact flow of each individual equation $\dot{y} = f^{[\nu]}(y)$, $\nu = 1, \dots, N$, preserves the first integral I. We then note that numerical methods formed by composition of such flows also preserve 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. The next theorem states that they are the only ones.

THEOREM 3.6 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 3.5, 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 Murua (2006). □

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 $f^{[\nu]}$, $\nu = 1, \ldots, N$. A B-series $B(\beta)$ with coefficients β satisfying $\beta(e) = 0$,

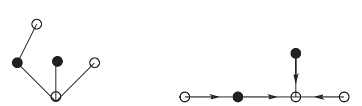
$$\sum_{t \in \mathscr{T}} \frac{h^{|t|}}{\sigma(t)} \beta(t) F(t),$$

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

$$\sum_{t \in \mathscr{T}} \frac{h^{|t|}}{\sigma(t)} \beta(t) \mathrm{div}(F(t)) = 0. \tag{4.1}$$

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

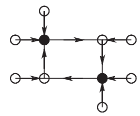
4.1.1 *Aromatic trees.* In order to conveniently represent $\mathrm{div}(F(t))$ for $t \in \mathscr{T}$, we introduce the following 'aromatic' trees, which are certain connected oriented graphs with one cycle. Before defining them, we observe that coloured rooted trees can be interpreted as connected oriented graphs with coloured vertices as follows: Given $t \in \mathscr{T}$, 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 $i \in V \backslash \{r\}$, there exists a unique sequence of vertices $j_1, \ldots, j_m \in V$ ($m \geqslant 1$) such that $(i, j_1), (j_1, j_2), \ldots, (j_{m-1}, j_m), (j_m, r) \in E$. 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.



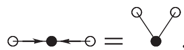
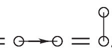
Similarly, a forest $t_1 \cdots t_m$ of coloured rooted trees can be identified with a coloured oriented graph whose connected components are identified with the rooted trees $t_1, \ldots, t_m$.

DEFINITION 4.1 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 ($t_1, \ldots, t_m \in \mathscr{T}$). If the arcs of o that form the cycle go from the root of t_i to the root of t_{i+1} ($i = 1, \ldots, m-1$) 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 $i \in \{2, \ldots, m\}$. The order $|o|$ of an aromatic tree $o = (t_1 \cdots t_m)$ is the number of its vertices, i.e. $|o| = |t_1| + \cdots + |t_m|$. The set of aromatic trees is denoted $\mathscr{AT}$ and the set of nth order aromatic trees $\mathscr{AT}_n$.

EXAMPLE 4.2 For the aromatic tree

$o =$  ,

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

$t_1 =$  , $t_2 =$  .

DEFINITION 4.3 For any aromatic tree $o = (t_1 \cdots t_m) \in \mathscr{AT}$, $C(o)$ is the unordered list of trees obtained from o by breaking any edge of the cycle. If we denote for $i = 1, \ldots, m$, $s_i = t_i \circ t_{i+1} \circ \cdots \circ t_m \circ t_1 \circ \cdots \circ t_{i-1}$, where the grafting operation is meant to operate from right to left, then

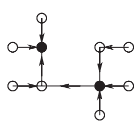
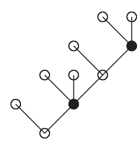
$$C(o) = \{s_1, \ldots, s_m\}. \tag{4.2}$$

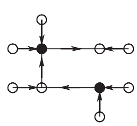
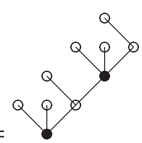
Now, let π_m be the circular permutation of $\{1, \ldots, m\}$ and let θ be

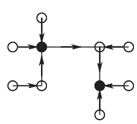
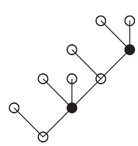
$$\theta = \#\left\{ l \in \{0, \ldots, m-1\} \colon \left(t_{\pi_m^l(1)}, \ldots, t_{\pi_m^l(m)}\right) = (t_1, \ldots, t_m)\right\},$$

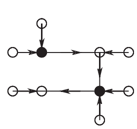
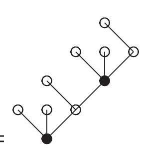
so that, for each i, there are θ copies of s_i in the list $C(o)$. Then, the symmetry coefficient of o is defined as $\sigma(o) = \theta \prod_i \sigma(t_i)$.

EXAMPLE 4.4 Consider again the aromatic tree o and the coloured rooted trees t_1 and t_2 in Example 4.2. 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 4.3, $C(o) = \{s_1, s_2, s_3, s_4\}$, where

$s_1 =$  $=$  $= t_2 \circ t_1 \circ t_2 \circ t_1,$

$s_2 =$  $=$  $= t_1 \circ t_2 \circ t_1 \circ t_2,$

$s_3 =$  $=$  $= t_2 \circ t_1 \circ t_2 \circ t_1,$

$s_4 =$  $=$  $= t_1 \circ t_2 \circ t_1 \circ t_2.$

For $t = [t_1, \dots, t_l]_\nu \in \mathscr{T}$, we shall use the notations of Araújo *et al.* (1997):

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

so that

$$\frac{\mathrm{d}F(t)}{\sigma(t)} = \frac{F^*(t)}{\sigma(t)} + \sum_{t_1 \circ t_2 \circ \cdots \circ t_m = t} \frac{F^*(t_1)}{\sigma(t_1)} \frac{F^*(t_2)}{\sigma(t_2)} \cdots \frac{F^*(t_m)}{\sigma(t_m)}. \tag{4.3}$$

DEFINITION 4.5 (Elementary divergence) The divergence $\mathrm{div}(o)$ associated with an aromatic tree $o = (t_1 \cdots t_m)$ is defined by

$$\mathrm{div}(o) = \mathrm{Tr}(F^*(t_1) \cdots F^*(t_m)). \tag{4.4}$$

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

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

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

REMARK 4.6 An alternative way of defining $\mathrm{div}(o)$ for an aromatic tree o is as follows: Given $o \in \mathscr{A}\mathscr{T}$, 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 $\xi \colon V \to \{1, \dots, N\}$, and the set of arcs $E \subset V \times V$. Let for each $i \in V$ denote $g_i = f^{[\nu]i}_{j_1,\dots,j_l}$, where $\nu = \xi(i)$ (the colour of the vertex i), $\{j_1, \dots, j_l\} = \{j \in V \colon (j, i) \in E\}$, and $f^{[\nu]i}_{j_1,\dots,j_l}(y)$ is the partial derivative of the ith component of $f^{[\nu]}(y)$ 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

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

4.1.2 *Divergence-free conditions and first consequences.* We are now in a 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 $\mathrm{div}(f^{[\nu]}) = 0$ for all $\nu = 1, \dots, N$, $\mathrm{Tr}(F^*(t)) = 0$ for all $t \in \mathscr{T}$. We thus have, by taking (4.3) into account,

$$\begin{aligned}
\mathrm{div}(B(\beta)) &= \sum_{t \in \mathscr{T}} \beta(t) \frac{h^{|t|}}{\sigma(t)} \mathrm{div}(F(t)) = \sum_{t \in \mathscr{T}} \beta(t) h^{|t|} \mathrm{Tr}\left(\frac{\mathrm{d}F(t)}{\sigma(t)}\right) \\
&= \sum_{t \in \mathscr{T}} \beta(t) h^{|t|} \sum_{m \geqslant 2} \sum_{t_1 \circ \cdots \circ t_m = t} \mathrm{Tr}\left(\frac{F^*(t_1)}{\sigma(t_1)} \frac{F^*(t_2)}{\sigma(t_2)} \cdots \frac{F^*(t_m)}{\sigma(t_m)}\right) \\
&= \sum_{t \in \mathscr{T}} \beta(t) h^{|t|} \sum_{m \geqslant 2} \sum_{t_1 \circ \cdots \circ t_m = t} \frac{\mathrm{div}((t_1 \cdots t_m))}{\sigma(t_1) \cdots \sigma(t_m)} \\
&= \sum_{n \geqslant 1} h^n \sum_{o \in \mathscr{A}\mathscr{T}_n} \left(\sum_{t \in C(o)} \beta(t)\right) \frac{\mathrm{div}(o)}{\sigma(o)}.
\end{aligned}$$

THEOREM 4.7 A modified field given by the B-series $B(\beta)$ is divergence free up to order p if the following condition is satisfied:

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

THEOREM 4.8 Condition (4.6) is a necessary condition for a vector field to be divergence free.

Proof. We will prove that, given $o \in \mathscr{AT}$ with $|o| = n$, there exist divergence-free vector fields $f^{[\nu]}\colon \mathbb{R}^n \to \mathbb{R}^n$, $\nu = 1, \ldots, N$, and $y_0 \in \mathbb{R}^n$ such that $\operatorname{div}(o)(y_0) = 1$ and for arbitrary $\hat{o} \in \mathscr{AT}\backslash\{o\}$, $\operatorname{div}(\hat{o})(y_0) = 0$.

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

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

Each such vector field $f^{[\nu]}$ is divergence free, as the main diagonal of its Jacobian matrix is identically null. The required result then follows, by taking Remark 4.6 into account, from the observation that, given $i, j_1, \ldots, j_l \in V = \{1, \ldots, n\}$, $f^{[\nu]i}_{j_1,\ldots,j_l}(y_0) \neq 0$ if and only if $\{j_1, \ldots, j_l\}$ ($j_1, \ldots, j_l$ being distinct) coincides with the set $\{j \in V\colon (j, i) \in E\}$. $\square$

LEMMA 4.9 The conditions for two and three 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

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

and

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

respectively.

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

$$b(t_1 \circ t_2 \circ t_3) = -b((t_2 \circ t_3) \circ t_1),$$

$$b(t_2 \circ t_3 \circ t_1) = -b((t_3 \circ t_1) \circ t_2),$$

$$b(t_3 \circ t_1 \circ t_2) = -b((t_1 \circ t_2) \circ t_3),$$

it can be rewritten as

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

which, together with (4.7), is the condition obtained in Chartier *et al.* (2006) 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 condition (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 $f^{[1]}, \ldots, f^{[N]}$ is trivially volume preserving (as the Lie bracket of divergence-free vector fields is also divergence free). We have already stated the following result on the nonexistence of nontrivial B-series methods preserving the volume.

THEOREM 4.10 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 $f^{[1]}, \ldots, f^{[N]}$.

Proof. This is a direct consequence of Lemma 4.9 and Theorem 3.6. □

DEFINITION 4.11 Consider an aromatic tree $o = (t_1 \cdots t_m)$. If we remove $1 \leqslant k \leqslant m$ 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 Section 4.2.

THEOREM 4.12 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 $1 \leqslant n \leqslant p$:

$$\forall\, o = (t_1 \cdots t_m) \in \mathscr{A}\mathscr{T}_n, \quad \sum_{k=1}^{m} (-1)^{k+1} \sum_{u \in C_k(o)} \alpha(u) = 0. \tag{4.9}$$

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

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

According to Lemma 2.17, we have for $\alpha_\tau = e^{\tau\beta}$ as defined in (2.4)

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

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

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

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

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

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

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

or, equivalently,

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

which after integration leads to the stated result. □

4.2.1 *Conditions for additive RK methods.* In this section, we consider additive RK methods as described in Araújo *et al.* (1997). Denoting the coefficients by $(a_{i,j}^{[1]}, b_i^{[1]}), \ldots, (a_{i,j}^{[N]}, b_i^{[N]})$, we can define recursively

$$\Phi(\bullet_\nu) = (1, \ldots, 1)^{\mathrm{T}} \in \mathbb{R}^s, \tag{4.12}$$

$$\Phi([t_1 \cdots t_m]_\nu) = \prod_{i=1}^{m} A^{[\mu(t_i)]} \Phi(t_i). \tag{4.13}$$

We then have $\alpha([t_1 \cdots t_m]_\nu) = (b^{[\nu]})^{\mathrm{T}} \Phi(t_i)$. Now, consider two trees t_1 and t_2 in $\mathscr{T}$. 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 $t_1, \ldots, t_m$ of $\mathscr{T}$, it becomes

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

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

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

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

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

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

DEFINITION 4.13 An aromatic multi-index $\rho = (i_1^{[\nu_1]} \cdots i_m^{[\nu_m]})$ is an oriented cycle where the vertices of the cycle are the 'coloured' indices $i_1^{[\nu_1]}, i_2^{[\nu_2]}, \ldots, i_m^{[\nu_m]}$. We denote by

$$C_1(\rho) = \{(i_1^{[\nu_1]}, \ldots, i_m^{[\nu_m]}), (i_2^{[\nu_2]}, \ldots, i_m^{[\nu_m]}, i_1^{[\nu_1]}), \ldots\}$$

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

$$C_2(\rho) = \{((i_2^{[\nu_2]}, i_3^{[\nu_3]}), (i_4^{[\nu_4]}, \ldots, i_m^{[\nu_m]}, i_1^{[\nu_1]})), \ldots\}$$

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

DEFINITION 4.14 Given an arbitrary ordered coloured multi-index $\varpi = i_1^{[\nu_1]} \cdots i_l^{[\nu_l]}$, we define

$$\psi(i_1^{[\nu_1]} \cdots i_l^{[\nu_l]}) := b_{i_1}^{[\nu_1]} a_{i_1 i_2}^{[\nu_2]} \cdots a_{i_{l-1} i_l}^{[\nu_l]},$$

and if $\upsilon = (\varpi_1, \ldots, \varpi_k)$ is a k-tuplet of ordered multi-indices, then

$$\psi(\upsilon) = \prod_{j=1}^{k} \psi(\varpi_j).$$

Then, the volume-preserving condition for the m-cycle $\rho = (i_1^{[\nu_1]} \cdots i_m^{[\nu_m]})$ reads

$$\sum_{k=1}^{m} (-1)^{k+1} \sum_{\upsilon \in C_k(\rho)} \psi(\upsilon) = 0 \quad \text{for each } (i_1^{[\nu_1]}, \ldots, i_m^{[\nu_m]}) \in \{1, \ldots, s\}^m. \tag{4.14}$$

It can be straightforwardly obtained from the conditions for the m-cycles $o = (t_1 \cdots t_m)$ by letting $t_1, \ldots, t_m$ be arbitrary trees of colours, respectively, $\nu_1, \ldots, \nu_m$. As a matter of fact, each matrix $X_l = \mathrm{diag}(\Phi(t_l))$ then spans the whole set of diagonal matrices and the choice $(X_l)_{r,r} = \delta_{r,i_l}$ leads to (4.14).

EXAMPLE 4.15
- For the coloured multi-index $\rho = (i^{[\nu_1]} j^{[\nu_2]})$, we obtain the conditions

$$b_i^{[\nu_1]} a_{ij}^{[\nu_2]} + b_j^{[\nu_2]} a_{ji}^{[\nu_1]} - b_i^{[\nu_1]} b_j^{[\nu_2]} = 0, \quad \nu_1, \nu_2 = 1, 2, \ \ i, j = 1, \ldots, s, \tag{4.15}$$

  i.e. the symplecticity conditions for additive RK methods (Araújo *et al.*, 1997).
- For the cycle $\rho = (i^{[\nu_1]} j^{[\nu_2]} k^{[\nu_3]})$, we get

$$b_i^{[\nu_1]} a_{ij}^{[\nu_2]} a_{jk}^{[\nu_3]} + b_j^{[\nu_2]} a_{jk}^{[\nu_3]} a_{ki}^{[\nu_1]} + b_k^{[\nu_3]} a_{ki}^{[\nu_1]} a_{ij}^{[\nu_2]} - b_i^{[\nu_1]} b_j^{[\nu_2]} a_{jk}^{[\nu_3]} - b_j^{[\nu_2]} b_k^{[\nu_3]} a_{ki}^{[\nu_1]} - b_k^{[\nu_3]} b_i^{[\nu_1]} a_{ij}^{[\nu_2]}$$
$$+ b_i^{[\nu_1]} b_j^{[\nu_2]} b_k^{[\nu_3]} = 0, \quad \nu_1, \nu_2, \nu_3 = 1, \ldots, 3, \ \ i, j, k = 1, \ldots, s.$$

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

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

  which has no other real solution than $b_1 = b_2 = \cdots = b_s = 0$. This condition is by itself sufficient to prove that there exist no volume-preserving RK methods and as a consequence that no RK method can preserve polynomial invariants of degree greater than or equal to 3 (see Calvo *et al.*, 1997; Zanna, 1998; Hairer *et al.*, 2002, Theorem IV 3.3.).

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 this section, we consider three particular cases where the vector fields $f^{[\nu]}$ $(\nu = 1, \ldots, N)$ have additional structure such that volume-preserving B-series methods exist apart from the trivial case of composition of volume-preserving flows.

The first case we consider is when each $f^{[\nu]}$ 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 Araújo *et al.* (1997).

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 Hairer *et al.*, 2002). 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 could be obtained for further generalizations of divergence-free systems split in $N \geqslant 4$ parts without any difficulty.

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

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

Now, let us consider the transposition operator τ defined on $\mathscr{A}\mathscr{T}$ as follows:

$$\forall\, o = (t_1 \cdots t_k) \in \mathscr{A}\mathscr{T}, \quad \tau(o) = (t_k t_{k-1} \cdots t_1). \tag{4.18}$$

Due to relation (4.17), we have

$$\forall\, o = (t_1 \cdots t_k) \in \mathscr{A}\mathscr{T}, \quad \mathrm{div}(o) = (-1)^k \mathrm{div}(\tau(o)). \tag{4.19}$$

This can be easily seen by considering the following identity:

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

THEOREM 4.16 Suppose that f is a sum of Hamiltonian parts (in possibly noncanonical form, i.e. K is just assumed to be an invertible skew-symmetric matrix) $f^{[\nu]} = K^{-1}\nabla H^{[\nu]}$. If the Hamiltonian conditions on the modified vector field $B(b)$,

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

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

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

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

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

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

Now, consider a tree $u \in C(o)$, for instance, $u = t_1 \circ t_2 \circ \cdots \circ t_k$. The tree $v = t_k \circ t_{k-1} \circ \cdots \circ t_1$ 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 the distance between their roots is $k-1$. Hence,

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

and condition (4.22) is satisfied. $\square$

4.3.2 *Two-cycle systems.* In this section, we consider the special situation of systems of the form

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

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

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

with

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

Note that partitioned RK 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 $\mathscr{T}$ need to be considered. If $t = [t_1, \ldots, t_m]_\bullet$, then $F(t)$ vanishes as soon as one of the t_i values 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 $u = [v_1, \ldots, v_m]_\bullet$ and $v = [u_1, \ldots, u_n]_\circ$ have, respectively, a black and a white root, $F^*(u)$ and $F^*(v)$ have the following forms:

$$F^*(u) = \frac{\partial^{m+1} f^{[1]}}{\partial(p,q)^{m+1}} (F(v_1), \ldots, F(v_m)) = \begin{pmatrix} 0 & \eta(p,q) \\ 0 & 0 \end{pmatrix},$$

$$F^*(v) = \frac{\partial^{n+1} f^{[2]}}{\partial(p,q)^{m+1}} (F(u_1), \ldots, F(u_m)) = \begin{pmatrix} 0 & 0 \\ \mu(p,q) & 0 \end{pmatrix},$$

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

LEMMA 4.17 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 $\operatorname{div}(o)$ 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 $\operatorname{div}(o) = 0$. □

THEOREM 4.18 A one-stage additive RK 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 $\rho = (i_1^{[1]} \cdots i_{2l}^{[2]})$ composed of $2l$ indices with colours in black/white order and let $v = (\varpi_1, \ldots, \varpi_k) \in C_k(\rho)$. Since all quantities are scalar, the indices $i_1^{[1]}, \ldots, i_{2l}^{[2]}$ take the value 1. Hence, if k_1 and k_2 denote the number of cuts before, respectively, a black and a 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

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

i.e.

$$(\theta_1 - 1)(\theta_2 - 1) = \theta_1\theta_2 \Longleftrightarrow \theta_2 = 1 - \theta_1. \tag{4.27}$$

□

THEOREM 4.19 Two-stage symplectic RK methods are volume preserving for separable systems of the form (4.24).

Proof. Consider a two-stage RK method with coefficient matrix $A \in \mathbb{R}^{2\times 2}$ and $b \in \mathbb{R}^2$. One of the following two situations occurs: either $\Phi(\bullet) = e$ and $\Phi([\bullet]) = Ae := c$ are linearly independent or for all trees $t \in \mathscr{T}$, $\Phi(t)$ 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 $t \in \mathscr{A}\mathscr{T}$. The discussion in Section 4.2.1 shows that (4.9) holds for a given $m \geqslant 2$ and for all $o = (t_1 \cdots t_m) \in \mathscr{A}\mathscr{T}$ if it holds in the particular case where $t_1, \ldots, t_m \in \{\bullet, \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}\}$.

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 $o = (t_1 \cdots t_{2m})$ with an even number of trees chosen in the set $\{\bullet, \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}\}$:

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

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

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

One can easily check that condition (4.28) is automatically satisfied provided that $t_1, \ldots, t_{2m} \in \{\bullet, \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}\}$.

Following the proof of Theorem 4.12 in the particular case where $t_1, \ldots, t_{2m} \in \{\bullet, \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}\}$, one observes that $\bar{\Delta}(t_{\pi^l(1)}) \circ \cdots \circ \bar{\Delta}(t_{\pi^l(m)})$ is a linear combination of terms of the form (4.11), with $z_1, \ldots, z_{2m} \in \{\bullet, \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}\}$ (this is due to the fact that $\bar{\Delta}(\bullet) = e \otimes \bullet$ and $\bar{\Delta}(\begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}) = e \otimes \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix} + \bullet \otimes \bullet$). We thus have that as (4.28) holds whenever $t_1, \ldots, t_{2m} \in \{\bullet, \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}\}$, the volume-preserving condition (4.9) holds for $o = (t_1, \ldots, t_{2m})$ if $t_1, \ldots, t_{2m} \in \{\bullet, \begin{smallmatrix}\bullet\\ \vert\\ \bullet\end{smallmatrix}\}$, which concludes the proof. $\square$

4.3.3 *Three-cycle systems.* In this section, we consider the special situation of systems of the form

$$\begin{cases} \dot{p} = \mathscr{F}(q), \\ \dot{q} = \mathscr{G}(r), \\ \dot{r} = \mathscr{H}(p), \end{cases} \tag{4.29}$$

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

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

and consider three 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 $\mathscr{A}\mathscr{T}$ need to be considered: if $t = [t_1, \ldots, t_m]_\bullet$, then $F(t)$ vanishes as soon as one of the t_i values 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 $w = [u_1, \dots, u_o]_\square$ have, respectively, a black, a white and a box root, $F^*(u)$, $F^*(v)$ and $F^*(w)$ have the following forms:

$$F^*(u) = \frac{\partial^{m+1} f^{[1]}}{\partial(p,q,r)^{m+1}}(F(v_1), \dots, F(v_m)) = \begin{pmatrix} 0 & \eta(p,q,r) & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$F^*(v) = \frac{\partial^{n+1} f^{[2]}}{\partial(p,q,r)^{n+1}}(F(w_1), \dots, F(w_n)) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mu(p,q,r) \\ 0 & 0 & 0 \end{pmatrix},$$

$$F^*(w) = \frac{\partial^{n+1} f^{[3]}}{\partial(p,q,r)^{n+1}}(F(u_1), \dots, F(u_o)) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \xi(p,q,r) & 0 & 0 \end{pmatrix},$$

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

LEMMA 4.20 Let o be an aromatic tree of the form $o = (t_1 \cdots t_m)$. If there exists an index i in $\{1, \dots, m\}$ for which the three consecutive trees t_i, t_{i+1} and t_{i+2} (or t_{m-1}, t_m and t_1 if $i = m-1$ or t_m, t_1 and t_2 if $i = m$) have roots that are not in the order black/white/box, then the corresponding elementary divergence $\operatorname{div}(o)$ is zero. In particular, if $m = 3l+1$ or $m = 3l+2$, then $\operatorname{div}(o)$ 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 no 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 do not have their roots with colours in the order black/white/box, we thus get $\operatorname{div}(o) = 0$. In particular, if $m = 3l+1$ or $m = 3l+2$, then there is necessarily such a sequence of three consecutive trees and $\operatorname{div}(o) = 0$. $\square$

THEOREM 4.21 A one-stage additive RK 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,

$$(\theta_1 - 1)(\theta_2 - 1)(\theta_3 - 1) = \theta_1\theta_2\theta_3. \tag{4.30}$$

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

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

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

$$\binom{l}{k_1}\binom{l}{k_2}\binom{l}{k_3} \tag{4.31}$$

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

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

i.e. if (4.30) holds. □

EXAMPLE 4.22 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

$$p_1 = p_0 + h\mathscr{F}\left(\frac{q_1 + q_0}{2}\right),$$

$$q_1 = q_0 + h\mathscr{G}(r_1),$$

$$r_1 = r_0 + h\mathscr{H}(p_0)$$

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

$$P = p_0 + \tfrac{h}{3}\mathscr{F}(Q), \quad p_1 = p_0 + h\mathscr{F}(Q),$$

$$Q = q_0 + \tfrac{4h}{3}\mathscr{G}(R), \quad q_1 = q_0 + h\mathscr{G}(R),$$

$$R = r_0 + \tfrac{h}{3}\mathscr{H}(P), \quad p_1 = p_0 + h\mathscr{H}(P)$$

and is not explicit.

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