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B-series methods cannot be volume-preserving *

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Abstract.

Volume preservation is one of the qualitative characteristics common to many dynamical systems. However, it has been proved by Kang and Shang that e.g. Runge–Kutta (RK) methods can not preserve volume for all linear source-free ODEs (let alone nonlinear ODEs). On the other hand, certain so-called Exponential Runge–Kutta (ERK) methods *do* preserve volume for all linear source-free ODEs. Do such ERK methods perhaps also preserve volume for all nonlinear ODEs? Here we prove that the answer to this question is negative; B-series methods (which include RK, ERK and several more classes of methods) cannot preserve volume for all source-free ODEs. The proof is presented via the theory of K-loops, which is an extension of the theory of classical rooted trees.

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1 Introduction

Volume preservation as a geometric property can be encountered in a large class of dynamical systems with many applications, for example, it underlies ergodic theory and thus statistical mechanics, and it appears in the tracking of particles in incompressible fluid flow. See [7, 15] and many references therein for recent reviews which discuss the numerical conservation of phase-space volume as well as many other geometric properties.

One of the common techniques to preserve volume is by using splitting methods [12]. This involves splitting a volume-preserving vector field $f(y)$ into a sum of essentially two-dimensional Hamiltonian vector fields [4, 12] before any integration is done.

On the other hand, Kang and Shang in [4] show that for a general (linear) source-free differential system of more than two dimensions, it is not possible to

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preserve volume by *direct* integration using classical methods (e.g. RK methods). This was done by showing that there exists no consistent approximation to the exponential function sending $\mathfrak{sl}(n)$ to $\mathrm{SL}(n)$, other than the exponential function itself.

However, if the source-free ODE is of the form

$$\dot{y} = Ay + b,$$

where $A \in \mathfrak{sl}(n)$ and $y, b \in \mathbb{R}^n$, then it is known that exponential integrators such as the explicit ERK methods of Hochbruck, Lubich and Selhofer [9, 10] produce exact solutions for linear ODEs and hence such numerical methods are volume-preserving for linear source-free problems. Such methods belong to a more general class of numerical integration methods known as B-series methods.

In this paper, we consider whether volume-preservation is possible for *general* source-free ODEs of more than two dimensions, and in particular, we wish to consider volume-preservation by B-series methods. The result is presented using the theory of *K-loops,* an extension to the classical theory of rooted trees [1]. Note that a similar result has been recently derived independently and using a different approach by Chartier and Murua in [3]. They show that a volume-preserving numerical method must also preserve all first integrals, and that the solution from a B-series method which preserves all cubic polynomial invariants is formally the exact flow of the vector field. As a consequence of the connection between cubic invariants and volume, no volume-preserving B-series method can exist.

2 Modified differential equations for B-series methods

Suppose that a system of ordinary differential equations is of the form

$$\dot{y} = f(y).$$

In classical numerical analysis, the numerical solution y_{n+1} (where n is the number of steps) of a numerical method can usually be represented by a series expansion in terms of the elementary differentials (derivatives) of $f(y)$. They in turn can be represented by rooted trees $t \in T$, where T is the set of all rooted trees, excluding the empty tree $\emptyset$, see [1]. Based on rooted trees, we can define the B-series [7].

DEFINITION 2.1. *For a mapping $a : T \cup \emptyset \to \mathbb{R}$, a formal series of the form*

$$B(a)(y) = a(\emptyset)y + \sum_{t \in T} \frac{h^{r(t)}}{\sigma(t)} a(t) F(t)(y),$$

is called a B-series, where h is the stepsize of the method, $F(t)(y)$ is the elementary differential of the rooted tree $t \in T$, $\sigma(t)$ is the symmetry function, and $r(t)$ is the order of t.

The family of B-series methods refers to numerical integrators whose solution y_{n+1} can be expanded in a B-series by Definition 2.1. It encompasses most integrators ubiquitous in practical computations, e.g. Runge–Kutta methods [1], multiderivative methods [8] and Elementary Differential Runge–Kutta methods [13].

Let the numerical solution be denoted as $\Phi(y)$. This is an approximation to the exact solution $\varphi(y)$ of the vector field $f(y)$, and $\Phi(y)$ matches $\varphi(y)$ to the order p of the numerical integrator. Here, instead of studying the original differential equation $\dot{y} = f(y)$, we can consider $\Phi(y)$ as the *exact* solution (up to exponentially small terms), of the modified differential equation $\dot{y} = \widetilde{f}(y)$. The construction of $\widetilde{f}(y)$ belongs to the area of numerical analysis called backward error analysis [6, 7]. This modified differential equation is a perturbation of the original vector field, where the first term is $f(y)$ and the next term is the leading term of the local truncation error of the method. This implies that for an order p B-series method, perturbing terms involve elementary differentials starting from order $p+1$.

For a B-series method, the modified differential equation is given by [7],

$$\dot{y} = \widetilde{f}(y) = \sum_{t \in T} \frac{h^{r(t)-1}}{\sigma(t)} b(t) F(t)(y), \tag{2.1}$$

where $b : T \to \mathbb{R}$ is the coefficient of this modified differential equation, and $b(\bullet) = 1$. The calculations of $b : T \to \mathbb{R}$ for a B-series method with solution given by $B(a)(y)$ can be found in [7].

3 Volume-preserving B-series method

Suppose that the system of ordinary differential equations to be solved is source-free, i.e. that $f(y)$ satisfies the divergence-free condition,

$$\nabla \cdot f(y) = 0.$$

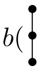
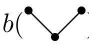
If an integrator – such as a RK method, or more generally, a B-series method – is to be volume-preserving, its modified differential equation must also be divergence-free,

$$\nabla \cdot \widetilde{f}(y) = 0.$$

From (2.1), the ith component of the modified differential equation is given by

$$\widetilde{f}^i(y) = f^i(y) + hb([\bullet]) f^i_j f^j(y) + h^2 b([[\bullet]]) f^i_j f^j_k f^k(y) + \frac{h^2}{2} b([\bullet,\bullet]) f^i_{jk} f^j f^k(y) + O(h^3),$$

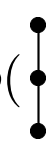
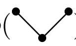
where elementary differentials are given in summation notation. Note that the superscript denotes vector field component, while subscript denotes derivatives in summation notation. We now apply the divergence-free condition to the above expression,

(3.1) $0 = f^i_i(y) + hb($$)[f^i_{ij}f^j + f^i_j f^j_i](y) + h^2 b($$)[f^i_{ij}f^j_k f^k + f^i_j f^j_{ik} f^k$
$+ f^i_j f^j_k f^k_i](y) + \frac{h^2}{2} b($$)[f^i_{ijk} f^j f^k + f^i_{jk} f^j_i f^k + f^i_{jk} f^j f^k_i](y)$
$+ O(h^3).$

Recall that the original vector field $f(y)$ is divergence-free. This implies

$$f^i_i(y) = f^i_{ij} f^j(y) = f^i_{ij} f^j_k f^k(y) = f^i_{ijk} f^j f^k(y) = \cdots = 0. \tag{3.2}$$

Hence (3.1) is reduced to,

(3.3) $0 = hb($$)f^i_j f^j_i(y) + h^2 b($$)[f^i_j f^j_{ik} f^k + f^i_j f^j_k f^k_i](y)$
$+ \frac{h^2}{2} b($$)[f^i_{jk} f^j_i f^k + f^i_{jk} f^j f^k_i](y) + O(h^3).$

We refer to the remaining terms in (3.3) as the *contracted elementary differentials*, and note that (3.3) must be satisfied if the associated B-series method is to preserve volume.

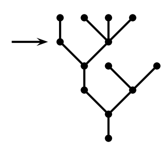
4 K-loops

We commence by defining K-loops, a central concept in our analysis.

Definition 4.1. *Given a rooted tree t with the vertices $v_1, v_2, \ldots, v_r$, where v_1 is the root, a K-loop is obtained from t by adding an edge extending from v_1 to a vertex v_j at a distance $K-1$ from the root.*

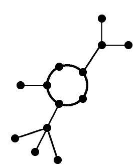
Note that a 1-loop occurs when the root is linked to itself.

As an example, consider the rooted tree



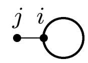
where we have singled out a vertex with an arrow. Once that vertex is joined to the root, we obtain the 5-loop

(4.1)



K-loops afford a convenient graphical representation of contracted elementary differentials. It follows from Section 3 that contracted elementary differentials arise from the divergence operator acting on $\widetilde{f}(y)$ in the divergence-free condition. This introduces an extra partial derivative (with respect to component y_i)

Table 4.1: Divergence operator acting on the elementary differential of order 2.

Elementary differential		Contracted elementary differentials		
	$\xrightarrow{\nabla\cdot}$		$+$	
$f^i_j f^j(y)$		$f^i_{ij} f^j(y)$		$f^i_j f^j_i(y)$
		1-loop		2-loop

to each elementary differential $F(t)(y)$. The K-loop is formed by joining the root (corresponding to y_i) with the vertex which is being partially differentiated with respect to y_i.

Each tree emerging from a loop retains its natural ordering, hence the concepts of "father" and "son" vertices will be clear within each subtree. Moreover, we assume clockwise ordering along the loop: each vertex is the father of its immediate clockwise neighbour.

For example, the elementary differential of order 2 is $f^i_j f^j(y)$. Once the divergence operator is applied, this yields two separate contracted elementary differentials by the product rule, and they are represented by the 1-loop and the 2-loop in Table 4.1.

Note that all 1-loops are trivial for a divergence-free vector field $f(y)$, because they represent the contracted elementary differentials in (3.2). As such, the smallest possible non-zero K-loops are the 2-loops, from order $r \geq 2$. Since trivial terms make no difference to our analysis, we henceforth disregard 1-loops and assume that $K \geq 2$.

4.1 Topologically equivalent $\boldsymbol{K}$*-loops*

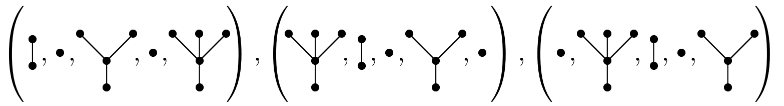
Definition 4.2. *Two K-loops $(t_1, t_2, \ldots, t_K)$ and $(s_1, s_2, \ldots, s_K)$ are* topologically equivalent *if there exists an integer m such that $s_{k+m} = t_k \bmod K$ for $k = 1, 2, \ldots, K$.*

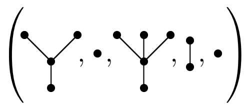
Each K-loop can be pictorially represented as a loop with K vertices and a tree emerging from each vertex. Given that the trees in question, arranged in *clockwise order* along the loop, are $t_1, t_2, \ldots, t_K$, we can alternatively represent the K-loop in the *subtree representation*

$$(t_1, t_2, \ldots, t_K).$$

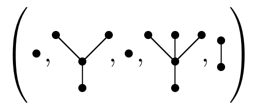
Note that there is arbitrariness in the choice of t_1 but all these choices are topologically equivalent.

To illustrate these concepts, we revisit the 5-loop (4.1). Its topologically equivalent subtree representations are





and



Topological equivalence is important since it corresponds to permutation of indices associated with vector field components in summation notation. For example

$$f^i_{jk} f^j_{lm} f^l_{in} F^k F^m F^n = f^j_{lk} f^l_{im} f^i_{jn} F^k F^m F^n.$$

Topologically equivalent K-loops form an equivalence class and it is convenient to be able to single out its representative (henceforth called the *standard representative*) in a unique manner. Let us assume thus that we are given an order "$\succ$" on trees (cf. [14] for an example, but for our purposes the specific order is not important). Given a subtree representation $(t_1, t_2, \ldots, t_K)$, we let $i \in \{1, \ldots, K\}$ such that

$$t_i \succeq t_j, \qquad j = 1, 2, \ldots, K.$$

If $t_i \succ t_j$ for all $j \neq i$, we let $(t_i, t_{i+1}, \ldots, t_K, t_1, \ldots, t_{i-1})$ be the subtree representative of the equivalence class. If there exists $m \neq i$ such that $t_i = t_m$, we compare t_{i+s} with t_{m+s} for $s = 1, 2, \ldots$, until $t_{i+s^*} \neq t_{m+s^*}$ for some s^*. If $t_{i+s^*} \succ t_{m+s^*}$, we choose the former representation, otherwise we take $(t_m, t_{m+1}, \ldots, t_K, t_1, \ldots, t_{m-1})$.

We adopt the convention that the "first" tree in a graphic representation of a K-loop is on the extreme left, with other trees in a clockwise order.

Table 4.2 displays all topologically non-equivalent K-loops from order 2 to order 4, their associated contracted elementary differentials, and the set of subtrees for each loop.

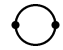
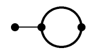
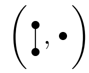
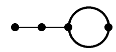
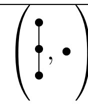
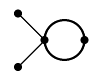
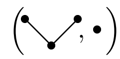
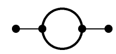
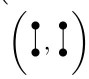
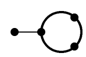
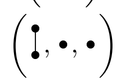
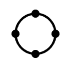
*4.2 Linearly independent **K**-loops*

It is now important to prove that K-loops are linearly independent of each other. (Note that when discussing independence of K-loops, we tacitly assume that they are acting on the space of divergence-free vector fields.) This implies that contracted elementary differentials associated with the K-loops can be treated as independent terms in the expansion of $\nabla \cdot \widetilde{f}(y) = 0$.

The proof of linear independence of K-loops will be by construction of special systems of differential equations. Firstly, the technique of scaling differential equation is used to prove that K-loops of *distinct* orders are linearly independent. Then, the proof for K-loops of the *same* order is presented, modelled on the familiar linear independence proof for rooted trees [2].

PROPOSITION 4.1. *K-loops of distinct orders are linearly independent.*

Table 4.2: Topologically non-equivalent K-loops from order 2 to order 4.

Order	K	Contracted elementary differential	K-Loop	Subtrees
2	2	$f^i_j f^j_i(y)$		$(\bullet, \bullet)$
3	2	$f^i_j f^j_{ik} f^k(y)$		
3	3	$f^i_j f^j_k f^k_i(y)$		$(\bullet, \bullet, \bullet)$
4	2	$f^i_j f^j_{ik} f^k_l f^l(y)$		
4	2	$f^i_j f^j_{ikl} f^k f^l(y)$		
4	2	$f^i_{jk} f^j_{il} f^k f^l(y)$		
4	3	$f^i_j f^j_k f^k_{il} f^l(y)$		
4	4	$f^i_j f^j_k f^k_l f^l_i(y)$		$(\bullet, \bullet, \bullet, \bullet)$

Proof. This proof is based on scaling of differential equations.

Let $C_n(f)$ and $C_{n+i}(f)$, where $n = 2, 3, \ldots$ and $i \in \mathbb{Z}^+$, be two non-identical (and non-trivial), contracted elementary differentials of orders n and $n+i$ respectively, applied to an *arbitrary* source-free differential equation f. From $\nabla \cdot \widetilde{f}(y) = 0$, assume that there exists a homogenous relation between C_n and C_{n+i} such that

$$\alpha C_n(f) + \beta C_{n+i}(f) = 0, \quad \text{for some } \alpha, \beta \in \mathbb{R} \setminus \{0\}. \tag{4.2}$$

Consider a source-free vector field V, itself the scaling of another source-free vector field v,

$$V = \delta v, \quad \text{where } \delta \in \mathbb{R}\backslash\{0, \pm 1\}. \tag{4.3}$$

Both systems of equations V and v must satisfy the homogenous relation in (4.2). By (4.3), this yields,

$$\begin{aligned} & \alpha C_n(V) + \beta C_{n+i}(V) = 0 \\ \Longrightarrow \quad & \alpha \delta^n C_n(v) + \beta \delta^{n+i} C_{n+i}(v) = 0, \end{aligned} \tag{4.4}$$

and

$$\begin{aligned} & \alpha C_n(v) + \beta C_{n+i}(v) = 0 \\ \Longrightarrow \quad & C_{n+i}(v) = -\frac{\alpha}{\beta} C_n(v). \end{aligned} \tag{4.5}$$

Substituting (4.5) into (4.4) yields

$$\alpha\delta^n(1-\delta^i)C_n(v) = 0. \tag{4.6}$$

From (4.6), it is observed that $\alpha = 0$, which implies $\beta = 0$ by (4.2). Hence, C_n and C_{n+i} are linearly independent of each other.

By the existence of such scaled source-free differential equations, it follows that all K-loops of distinct orders are linearly independent. □

If the K-loops are of the same order then the proof of their linear independence is modelled on the proof of the independence of elementary differentials in [2, 8]. Similarly to the classical proof, a source-free differential equation $f(y)$ can be constructed for each (equivalence class of) K-loops, such that when a contracted elementary differential evaluates $f(y)$, the result is non-zero only if the contracted elementary differential is associated with a K-loop which is *equivalent* to the K-loop for the corresponding vector field. Otherwise, the result is zero.

It is important to note that there exist other constructions of such special types of vector fields for each K-loop [18]. The important idea is that there is at least *one* such type which has the unique properties described above for each loop. Hence, there can be no linear relation between topologically non-equivalent K-loops in general, and the assumption that the contracted elementary differentials are linearly independent is valid.

PROPOSITION 4.2. *Topologically non-equivalent K-loops of the same order are linearly independent.*

The proof of Proposition 4.2 is presented in several parts, where the key idea is the construction of the special vector field for K-loops. This differential-equation construction in the discussion below is based on the construction in [2]. For a monotonically labelled [8] rooted tree $t \in T$ of order r, the system of differential equations constructed to prove its independence has dimension r. Each component of this system is represented by a unique vertex of t, such that each component is defined by the relation between its *father* vertex and the *son* vertices [2].

DEFINITION 4.3. *Let a K-loop, denoted L_K, be of order $r \geq K$ with standard representative $s^* = (t_1, t_2, \ldots, t_K)$. We denote by S_i the set of all the indices corresponding to sons of a vertex i of L_K.*

We associate with L_k the r-dimensional differential system,

$$\begin{aligned} \dot{y}_1 &= \prod_{n\in S_1} \frac{y_n}{\sum(L_K)} \\ \dot{y}_m &= \begin{cases} \prod\limits_{n\in S_m} y_n & \text{for } m \neq 1 \text{ and } S_m \neq \emptyset \\ 1 & \text{for } m \neq 1 \text{ and } S_m = \emptyset \end{cases}, \end{aligned} \tag{4.7}$$

with initial condition at $t = 0$ given by,

$$y(0) = (0, \ldots, 0).$$

The weight $\sum(L_K)$ *is given by*

$$\sum(L_K) = R(L_K)\sigma(t_1)\sigma(t_2)\cdots\sigma(t_K).$$

Here $R(L_K)$ *is the* order of the rotational symmetry *in the sequence of subtrees is denoted* $R(L_K)$*, and* $\sigma(t_i)$ *is the* symmetry *[1] of the rooted subtree* t_i*, for* $i = 1, \dots, K$[1].

Why is the weight $\sum(L_K)$ necessary? When a contracted elementary differential is applied to its system of differential equations from Definition 4.3, all of its indices $\{i, j, k, \dots\}$ in the differential are summed over, and the resulting number of non-zero terms in the summation depends on the symmetries of subtrees in the standard decomposition of L_K. Hence, $\sum(L_K)$ acts as a normalization. If all subtrees of L_K are unique then the number of non-zero terms in the evaluation is equal to the product $\sigma(t_1)\cdots\sigma(t_K)$ and $R(L_K) = 1$. But, once the subtrees are not unique, rotational symmetry in the sequence is possible. That is, i of the contracted elementary differential can start on more than one vertex in the cycle of the K-loop, resulting in non-zero terms. Hence, an extra factor of $R(L_K)$ representing this rotational symmetry is required.

Table 4.3 displays the source-free systems of differential equations for selected K-loops from order 2 to order 4.

Now, it can be shown that the existence of the source-free differential equations as described by Definition 4.3 is the key to proving that two topologically non-equivalent K-loops of the same order must be linearly independent, by the proposition stated below.

Proposition 4.3. *Consider the initial-value problem (4.7), associated with the K-loop L_K in accordance with Definition 4.3, at $t = 0$. All K-loops which are equivalent to L_K will evaluate the differential system to one at $t = 0$. A K-loop which is topologically non-equivalent to L_K will evaluate the same differential system to zero at $t = 0$.*

That is, if $\mathcal{L}$ denotes a K-loop of order r, and $F(\mathcal{L})(y)$ denotes the evaluation of the differential system by the contracted elementary differential associated with $\mathcal{L}$, then

$$F(\mathcal{L})(0) = \begin{cases} 1, & \mathcal{L} \text{ is in the equivalence class of } L_K, \\ 0, & \text{otherwise} \end{cases} .$$

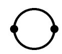
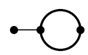
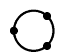
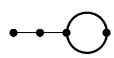
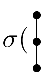
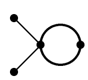
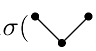
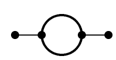
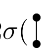
Proof. We apply a contracted elementary differential

$$\sum_{J_1,\dots,J_r=1}^{r} f^{J_1}_{T_{J_1}} f^{J_2}_{T_{J_2}} \cdots f^{J_r}_{T_{J_r}},$$

to the initial value problem in (4.7). Note that T_{J_i} is the set of sons of the integer index J_i, which runs from 1 to r in the summation. Hence, the search for a non-zero application of the contracted elementary differential to the initial

[1] Note that a slightly different vector field, e.g. without normalization factor, is used in [3].

Table 4.3: Selected K-loops from order 2 to order 4 and their associated source-free vector fields.

r	K-loop	$f(y)$	$\Sigma(L_K)$
2		$\dot{y}_1 = \frac{1}{2}y_2$ $\dot{y}_2 = y_1$	$\Sigma = 2\sigma(\bullet) = 2$
3		$\dot{y}_1 = y_2$ $\dot{y}_2 = y_1 y_3$ $\dot{y}_3 = 1$	$\Sigma = 1\sigma($$)\sigma(\bullet) = 1$
3		$\dot{y}_1 = \frac{1}{3}y_2$ $\dot{y}_2 = y_3$ $\dot{y}_3 = y_1$	$\Sigma = 3\sigma(\bullet)^3 = 3$
4		$\dot{y}_1 = y_2$ $\dot{y}_2 = y_1 y_3$ $\dot{y}_3 = y_4$ $\dot{y}_4 = 1$	$\Sigma = 1\sigma($$)\sigma(\bullet) = 1$
4		$\dot{y}_1 = \frac{1}{2}y_2$ $\dot{y}_2 = y_1 y_3 y_4$ $\dot{y}_3 = 1$ $\dot{y}_4 = 1$	$\Sigma = 1\sigma($$)\sigma(\bullet) = 2$
4		$\dot{y}_1 = \frac{1}{2}y_2 y_3$ $\dot{y}_2 = y_1 y_4$ $\dot{y}_3 = 1$ $\dot{y}_4 = 1$	$\Sigma = 2\sigma($$)^2 = 2$

value problem is equivalent to choosing an integer $m \in \{1, \ldots, r\}$ for J_i such that when the contracted elementary differential is applied to the vector field component $\dot{y}_m$ in (4.7), $J_i = m$ and

$$f^{J_i}_{T_{J_i}} = f^m_{T_m} \neq 0.$$

The rest of this proof examines the restriction on T_{J_i} such that the above evaluation is non-zero.

Suppose that in the terminology of (4.7), $S_m = \emptyset$. Then $\dot{y}_m \equiv 1$. In this case, the only contracted elementary differential which is non-zero, once applied to $\dot{y}_m$, must contain the integer index J_i which is chosen to be $J_i = m$, where $T_{J_i} = T_m = \emptyset$. So the contribution of this term is a factor of 1 and $S_m = T_{J_i}$.

Now, let us assume that $S_m = \{j_1, \ldots, j_s\} \neq \emptyset$ and $T_{J_i} = \{J_{\mu_1}, J_{\mu_2}, \ldots\}$.

Suppose that when the contracted elementary differential is applied to $\dot{y}_m$ we can choose the integer index $J_i = m$ and all sons to be $J_{\mu_1} = j_1, J_{\mu_2} = j_2, \ldots, J_{\mu_s} = j_s$ such that

$$S_m = T_{J_i}.$$

Then,

$$f^{J_i}_{T_{J_i}} = f^m_{j_1,\ldots,j_s} = \frac{\partial^s}{\partial y_{j_1} \cdots \partial y_{j_s}} \dot{y}_m = \frac{\partial^s}{\partial y_{j_1} \cdots \partial y_{j_s}} \prod_{k=1}^{s} y_{j_k} = 1.$$

Note that if the K-loop L_K has $\Sigma(L_K) > 1$ in the vector field construction, then it may be possible that J_i is one of several integer indices in the contracted elementary differential which can be set to integer m, and resulting in $T_{J_i} = S_m$. In this case,

$$f^{J_i}_{T_{J_i}} = f^m_{j_1,\ldots,j_s} = \frac{1}{\Sigma(L_K)} \neq 0.$$

Next, suppose that by setting the integer index $J_i = m$ when evaluating $\dot{y}_m$ with the contracted elementary differential, we are unable to choose the indices $J_{\mu_1}, J_{\mu_2}, \ldots$ in T_{J_i} such that this set is equivalent to the set $S_m = \{j_1, \ldots, j_s\}$. This restriction can occur if for example, J_{μ_1} is defined to be an integer $j_\nu \notin S_m$ for the evaluation of another vector field component $\dot{y}_n$ where $n \neq m$. For the integer index J_i, this means that,

$$S_m \neq T_{J_i}.$$

In this case there are two possibilities.

Firstly, assume that $J_{\mu_1} = j_\nu \in T_{J_i}$ but the integer $j_\nu \notin S_m$. Then once we apply $f^{J_i}_{T_{J_i}} = f^m_{T_m}$ to $\dot{y}_m$, we differentiate by a variable y_{j_ν} which does not feature in the equation. Hence the outcome is necessarily zero.

Alternatively, there exists an integer $j_\nu \in S_m$ such that $j_\nu \notin T_{J_i}$ (i.e. $J_{\mu_1} \neq j_\nu, J_{\mu_2} \neq j_\nu, \ldots$). Once we apply $f^{J_i}_{T_{J_i}} = f^m_{T_m}$ to the vector field component $\dot{y}_m$, the variable y_{j_ν} survives in the product and the latter becomes zero once the initial condition at $t = 0$ is substituted.

We deduce then that the only possibility for a non-zero application of the contracted elementary differential to the initial value problem at $t = 0$ is when

$$T_{J_i} = S_m, \quad \text{where } J_i = m \text{ and } m \in \{1, \ldots, r\}.$$

Now, to show that such integer index J_i ($\forall i = 1, \ldots, r$) must be distinct for $r \geq K > 1$, consider the following: K-loops are injective (i.e. each vertex of the K-loop has exact one father). Then a contracted elementary differential associated with this K-loop of order r has exactly r father vertices, denoted as superscripts given by the integer indices $\{J_1, \ldots, J_r\}$. Note that each index J_i also appears exactly once as a subscript, since the father vertex J_i must in turn, appear as the son of some other father vertex in the K-loop.

Suppose L_K is a K-loop of order $r = K$ and the vertices are labelled distinctly by integers $\{1, 2, \ldots, K\}$. Then in the contracted elementary differential which evaluates the vector field non-trivially, each integer $\{1, \dots, K\}$ must appear exactly once as a subscript and superscript in the differential. That is for example, $J_1 = 1, J_2 = 2, \dots, J_K = K$. This is because each vertex is the father of exactly one son. Hence all J_i for all $i = 1, \dots r$ are distinct when $r = K$ and $K \geq 2$.

Suppose now the order is $r = K + \delta$, where $\delta = 1, 2, \dots$. Then there are now extra integers $\{K+1, \dots, K+\delta\}$ which are the labels of the vertices of the subtrees attached to the loop of L_K. For the contracted elementary differential, there are now $K + \delta$ integer indices, of which $J_1 = 1, \dots, J_K = K$ denoting the vertices in the loop have been assigned. Hence we are left with integer indices $J_{K+1}, \dots, J_{K+\delta}$, of which their integer values are determined by the remaining $\{K+1, \dots, K+\delta\}$. This is because each vertex of the subtree must be joined to exactly one father, and they themselves can be considered as father vertices in their own right. Hence, all integer indices J_i must be distinct for $r \geq K$.

We have shown that the integer indices J_i must be distinct in the contracted elementary differential, hence the condition that $T_{J_i} = S_m$ for non-trivial evaluation covers all vertices of L_K. This occurs only if the K-loop associated with the contracted elementary differential is topologically equivalent to L_K which generates the initial value problem in (4.7).

Furthermore, such non-trivial evaluation must result in one, even for K-loops with $\Sigma(L_K) > 1$. This is because when the contracted elementary differential evaluates $\dot{y}_m$, the total number of possible choices for integer indices J_i and permutations of sons of J_i which can be set to integer $m \in \{1, \dots, r\}$ and the indices in the set S_m, is given by the normalisation $\Sigma(L_K)$. This concludes the proof.

□

We are now ready to return to the proof of Proposition 4.2.

Proof. [Proposition 4.2] By Definition 4.3 and Proposition 4.3, since there exists at least *one* type of source-free differential equations which result in non-zero solution only when the system is evaluated by a K-loop which is equivalent to L_K, any two K-loops of the *same* order which are topologically non-equivalent must be linearly independent of each other for an *arbitrary* source-free system of differential equation. □

Furthermore, as opposed to the classical proof of the independence of rooted trees in [2], Definition 4.3 cannot be used to prove that two non-equivalent K-loops of *distinct* orders are linearly independent. This is because certain contracted elementary differentials of integer multiples of order r also evaluate the same system of differential equations to one. For example, assume that a system is constructed for a K-loops of order r. By Proposition 4.3, the evaluation by L_K, to this system yields $F(L_K)(y) = 1$. However, for positive integer multiples of order r, contracted elementary differentials of the form $F(L_K)^n(y)$ (and all their permutations) are also non-trivial. Here, the superscript n denotes the product of n copies of $F(L_K)$. Hence, the technique of scaling differential equations is required to prove that K-loops of *distinct* orders are also linearly independent.

Combining Proposition 4.1 and Proposition 4.2 results in the following.

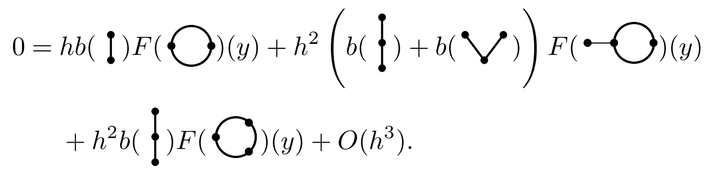
LEMMA 4.4. *All topologically non-equivalent K-loops must be linearly independent when evaluating arbitrary source-free vector fields.*

5 Coefficients of the volume-preserving *B*-series method

The impact of the divergence-free condition on the modified differential equation of a B-series method can be investigated using topological equivalence and linear independence of K-loops,

5.1 Linear system by the independence of $\boldsymbol{K}$*-loops*

Due to topological equivalence, the expansion $\nabla \cdot \widetilde{f}(y) = 0$ given in (3.3) can be rewritten by gathering the coefficients $b(t)$ of rooted trees t that lead to topologically equivalent K-loops. This yields

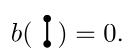


(5.1)

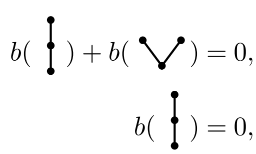
Note that $F(\cdot)(y)$ now denotes the evaluation of the original source-free ODE $f(y)$ by the associated contracted elementary differentials of the equivalence classes of K-loops.

For a general source-free system of differential equations, it is assumed that the contracted elementary differentials $F(\cdot)(y)$ in (5.1) are non-trivial. Furthermore, by Lemma 4.4, each term in (5.1) can be treated separately, resulting in one equation (involving the coefficients $b(t)$), for each K-loop. This set of linear equations is displayed in Table 5.1, from order 2 to order 5, along with their associated K-loops.

The coefficients $b(t)$ which satisfy the divergence-free condition can be solved by studying the linear equations for each order r. For example, for order two



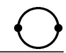
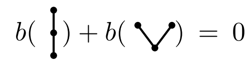
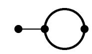
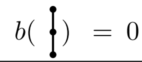
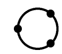
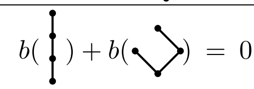
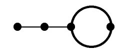
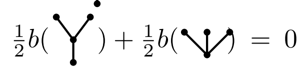
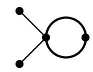
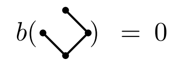
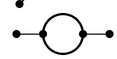
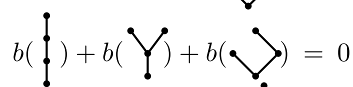
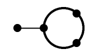
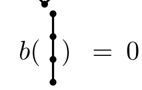
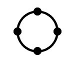
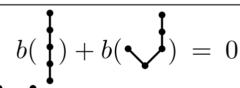
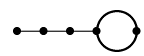
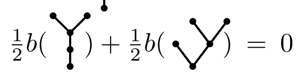
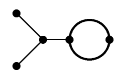
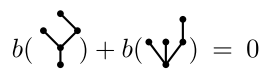
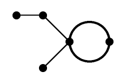
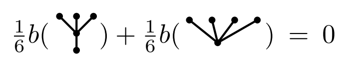
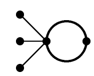
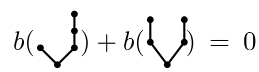
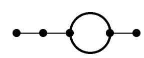
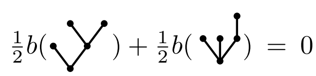
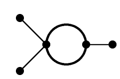
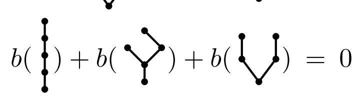
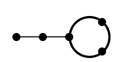
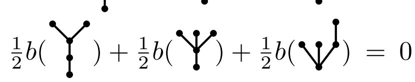
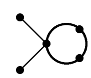
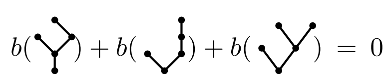
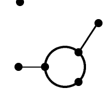
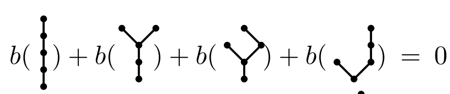
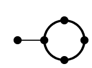
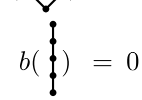
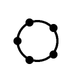
Similarly, for order three,



and we observe that the system is satisfied only when both coefficients for order-3 rooted trees are trivial.

We can continue in this vein for higher orders. However, the number of linear equations for each order corresponds to the number of K-loops, while the number of unknown coefficients $b(t)$ is the number of rooted trees for that order. So for higher order the linear system becomes overdetermined. For example, at order

Table 5.1: Linear equations for topologically non-equivalent K-loops.

Order	Linear Equations	K-loops
2		
3		
		
4		
		
		
		
		
5		
		
		
		
		
		
		
		
		
		
		

10, there are 1592 linear equations and just 719 rooted tree coefficients [18]. Hence the likelihood of non-trivial solutions $b(t)$ is very small. This argument, however, falls short of a formal proof.

It would have been useful if the above method of proof could be extended to *all* orders, but it is clear that it faces substantial difficulty since a general expansion of $\nabla \cdot \widetilde{f}(y) = 0$ can not be written for an infinite number of terms. So, recursive relations for the K-loops and their associated coefficients must be developed, and this is possible by considering in the first instance the relations between the linear equations from the 2-loops and symplectic conditions for a general B-series method.

5.2 2-loop equations and symplectic conditions

It was proved in Hairer's paper on the backward analysis of symplectic methods [5] that for a Hamiltonian differential equations $f(y)$ in the canonical form

$$\dot{y} = J^{-1}\nabla H(y),$$

where H is the Hamiltonian function, the modified differential equation in (2.1) is Hamiltonian if and only if

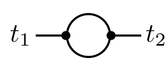
$$b(u \circ v) + b(v \circ u) = 0 \quad \text{for } u, v \in T. \tag{5.2}$$

Note that $\circ$ is the Butcher product [1], and $b : T \mapsto \mathbb{R}$ are the coefficients in the modified differential equation for the B-series method.

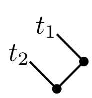
Interestingly, this condition corresponds precisely to linear 2-loop equations in Table 5.1 from Section 5.1. This holds for all orders $r \geq 2$, and we have the following lemma.

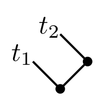
LEMMA 5.1. *Linear 2-loop equations from Section 5.1 are equivalent to the application of the symplectic condition given by* (5.2)*, to rooted trees* $u \circ v$ *and* $v \circ u \in T$ *where* $r(u) + r(v) \geq 2$*.*

PROOF. For order 2 it can be observed directly that the symplectic condition given by (5.2) results in the 2-loop equation for a rooted tree of order 2. For order $q \geq 3$ consider an equivalence class of 2-loops of the form



where $t_1, t_2 \in T \cup \{\emptyset\}$ are such that $r(t_1) + r(t_2) + 2 \geq 3$. Recall that the extra path forming the cycle in the K-loop always ends at the *root* of the original rooted tree t, where $r(t) = q$. Hence, one of the two vertices in the cycle of the 2-loop must be the root of t, and the 2-loop can be derived from at most two different rooted trees c and d, where $r(c) = r(d) = q$, namely

$c =$ 

and $d =$ 

.

As such, c and d must correspond to the same free tree $t_f =$ 

, and c differs from d by at most an adjacent root. Hence by topological equivalence of

K-loops, the coefficients of rooted trees c and d obey

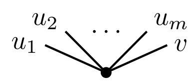
$$k_1 b(c) + k_2 b(d) = 0, \quad \forall k_1, k_2 \in \mathbb{R}.$$

The rest of this proof involves showing that $k_1 = k_2$ for rooted trees c and d so that the symplectic condition in (5.2) is recovered. We refer to [16, 17] for the theory of free (un-rooted) trees.

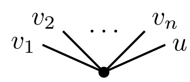
For $u, v \in T$ and $m, n \in \mathbb{Z}^+$, let $(u_1, \ldots, u_m)$ and $(v_1, \ldots, v_n)$ denote the remaining forest of rooted trees when the roots are removed from u and v [1], such that

$$u = [u_1, u_2, \ldots, u_m], \quad v = [v_1, v_2, \ldots, v_n].$$

Then rooted trees c and d can be defined as

$$c = u \circ v = [u_1, u_2, \ldots, u_m, v] :$$ 

,

$$d = v \circ u = [v_1, v_2, \ldots, v_n, u] :$$ 

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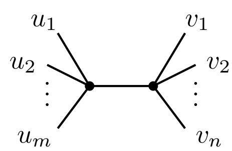
The corresponding free tree t_f at order q for both c and d is given by

$t_f =$ 

Because of (2.1), $\widetilde{f}(y)$ for the B-series method now contains two terms involving the two rooted trees c and d,

$$h^{q-1} \frac{b(c)}{\sigma(c)} F(c)(y) + h^{q-1} \frac{b(d)}{\sigma(d)} F(d)(y). \tag{5.3}$$

Once the divergence-free condition is imposed on $\widetilde{f}(y)$, elementary differentials $F(t)(y)$ (for rooted tree t) become contracted elementary differentials $F(\mathcal{L})(y)$ (for K-loop $\mathcal{L}$). Since the rooted trees c and d differ by an adjacent root, the 2-loop equation involving coefficients $b(c)$ and $b(d)$ is derived when the 2-loop $\mathcal{L}_c$ from tree c is topologically equivalent to the 2-loop $\mathcal{L}_d$ from tree d. That is,

$$\mathcal{L}_c = \mathcal{L}_d \quad \Longrightarrow \quad F(\mathcal{L}_c)(y) = F(\mathcal{L}_d)(y).$$

Hence, (5.3) can be rewritten in the form

$$h^{q-1} \left[\alpha(c) \frac{b(c)}{\sigma(c)} + \alpha(d) \frac{b(d)}{\sigma(d)} \right] F(\mathcal{L}_c)(y). \tag{5.4}$$

Note that $\alpha : T \to \mathbb{R}$ is an extra factor dependent on the symmetries of the rooted trees c and d, because it might be possible to construct multiple copies of isomorphic 2-loops from the same rooted tree. By linear independence of K-loops, (5.4) yields the 2-loop equation

$$\alpha(c)\frac{b(c)}{\sigma(c)} + \alpha(d)\frac{b(d)}{\sigma(d)} = 0. \tag{5.5}$$

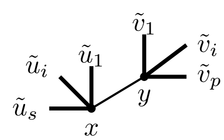
For Lemma 5.1 to hold, it is required that

$$\frac{\alpha(c)}{\sigma(c)} = \frac{\alpha(d)}{\sigma(d)}. \tag{5.6}$$

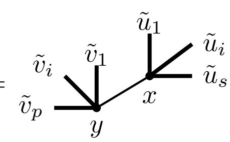
To demonstrate that (5.6) is true, the functions α and σ must be expressed in terms of the forests of rooted trees from c and d. To begin, let $u, v \in T$ be denoted as

$$u = [u_1, u_2, \ldots, u_m] = [\tilde{u}_1^{k_1}, \tilde{u}_2^{k_2}, \ldots, \tilde{u}_s^{k_s}],$$
$$v = [v_1, v_2, \ldots, v_n] = [\tilde{v}_1^{l_1}, \tilde{v}_2^{l_2}, \ldots, \tilde{v}_p^{l_p}],$$

where $\tilde{u}_1, \ldots, \tilde{u}_s$ and $\tilde{v}_1, \ldots, \tilde{v}_p$ are distinct rooted trees from the forests of $[u_1, \ldots, u_m]$ and $[v_1, \ldots, v_n]$. The positive integers $k_1, \ldots, k_s$ and $l_1, \ldots, l_p$ denote multiple copies of the *distinct* rooted trees $\tilde{u}_i$ and $\tilde{v}_j$, for $i = 1, \ldots, s$, and $j = 1, \ldots, p$, respectively [1]. Then, rooted trees c and d are given by

$c = u \circ v =$ 

and

$d = v \circ u =$ 

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where thick lines indicate trees that might be of nontrivial multiplicity. The root of u (and hence c) is denoted by x, and the root of v (and hence d) by y. To study the relations between c and d, it is useful to consider two separate cases: when $\tilde{u}_i \neq v$ for $i = 1, \ldots, s$; and when $\tilde{u}_i = v$ for some $i \in \{1, \ldots, s\}$.

For the rooted tree c, when $\tilde{u}_i \neq v$ for $i = 1, \ldots, s$, it is true that $\alpha(c) = 1$ with respect to vertex y and root x. Its symmetry is $\sigma(c) = \sigma(u)\sigma(v)$. Similarly for rooted tree d, the two cases are

1. If $\tilde{v}_i \neq u$ for $i = 1, \ldots, p$, then $\alpha(d) = 1$ with respect to vertex x and root y. Its symmetry is given by

$$\sigma(d) = \sigma(u) l_1! \sigma(\tilde{v}_1)^{l_1} \cdots l_p! \sigma(\tilde{v}_p)^{l_p} = \sigma(u)\sigma(v).$$

In this case

$$\frac{\alpha(d)}{\sigma(d)} = \frac{1}{\sigma(u)\sigma(v)} = \frac{\alpha(c)}{\sigma(c)}.$$

2. If $\tilde{v}_i = u$ for $i \in \{1, \ldots, p\}$, then $\alpha(d) = l_i + 1$ with respect to vertex x and root y. Its symmetry is given by

$$\sigma(d) = l_1!\sigma(\tilde{v}_1)^{l_1} \cdots (l_i + 1)!\sigma(\tilde{v}_i)^{l_i+1} \cdots l_p!\sigma(\tilde{v}_p)^{l_p}.$$

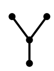
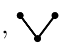
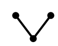
   In this case

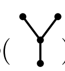
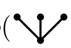
$$\begin{aligned}\frac{\alpha(d)}{\sigma(d)} &= \frac{l_i + 1}{l_1!\sigma(\tilde{v}_1)^{l_1} \cdots (l_i + 1)!\sigma(\tilde{v}_i)^{l_i+1} \cdots l_p!\sigma(\tilde{v}_p)^{l_p}} = \frac{1}{\sigma(v)\sigma(\tilde{v}_i)} \\ &= \frac{1}{\sigma(v)\sigma(u)} = \frac{\alpha(c)}{\sigma(c)}.\end{aligned}$$

Hence, (5.6) holds when $\widetilde{u}_i \neq v$ for $i = 1, \ldots, s$.

The second case, when $\widetilde{u}_i = v$ for some $i \in \{1, \ldots, s\}$, follows along similar lines, and it can be shown that (5.6) also holds. Hence, (5.5) is equivalent to the symplectic condition (5.2) applied to rooted trees $c = u \circ v$ and $d = v \circ u$ which differ by an adjacent root. □

Table 5.2 displays the 2-loop equations from order 2 to order 5, which can be extracted from Table 5.1. Conversely, by the application of the symplectic condition (5.2), it is possible to derive all 2-loop equations for orders $r \geq 2$. This is done by considering the standard decomposition of a rooted tree $t = (u, v)$, then constructing $c = u \circ v$ and $d = v \circ u$ by the Butcher product. For example, the following rooted tree at order 4 has the given standard decomposition [14],

 $= (\ \bullet\ ,$ $)$. Let $u = \ \bullet$ and $v =$ .

$\Longrightarrow\ b(u \circ v) + b(v \circ u) = b($  $) + b($$) = 0.$

5.3 *B-series coefficients via the recursive relations on free trees*

We know from the previous section that the 2-loop linear equations are the conditions for the modified differential equation to be Hamiltonian. Therefore, the modified vector field in (2.1) must be made up of Hamiltonian combinations of elementary differentials [13], and we can now rewrite $\widetilde{f}(y)$ accordingly. Once this modified differential equation is constructed, the divergence-free condition can be applied for volume-preserving B-series methods.

Hamiltonian combinations of elementary differentials defined in [13] are based on the (non-superfluous) free trees t_f of each order. Free trees $t_f \in F$ (where F denotes the set of all free trees) are the un-rooted trees, where the root of each tree is no longer distinguished from other vertices [16, 17]. If the free tree t_f is constructed by joining two copies of the same rooted tree by their roots, then this free tree is said to be *superfluous* [16]. Otherwise, it is non-superfluous.

Furthermore, the set of rooted trees generated by any non-superfluous free tree t_f sub-divides into two different parities [16], which can be denoted with "+" and "−" signs. For each non-superfluous free tree t_f the centroid vertex

[11] has a "+" sign. Likewise, vertices with an even number of shifts away from the centroid are denoted with "+" signs. All other vertices are assigned a "−" sign. According to the respective signs associated with the roots of the rooted trees, they can be separated into their respective + and − parity classes P_+ and P_-, respectively. Table 5.3 displays the free trees and their associated rooted trees from order 1 to order 5. Free trees without ± signs are superfluous.

Each non-superfluous free tree corresponds to a Hamiltonian combination of elementary differentials [13]. This linear combination is denoted $H(t_f)(y)$ for each t_f.

DEFINITION 5.1. *The Hamiltonian combination of elementary differentials $H(t_f)(y)$ of a non-superfluous free tree $t_f \in F$ is the linear combination*

$$H(t_f)(y) = \sum_{u \in P_+} \frac{1}{\sigma(u)} F(u)(y) - \sum_{v \in P_-} \frac{1}{\sigma(v)} F(v)(y),$$

where the sums are taken over all rooted trees $u, v \in T$ generated by the free tree $t_f \in F$ in the two parity classes P_+ and P_- of the rooted trees in T.

Table 5.4 displays the Hamiltonian combinations of elementary differentials of order 1 to 5.

Once the Hamiltonian combinations are constructed, the modified differential equation is given by

$$\dot{y} = \widetilde{f}(y) = f(y) + \sum_{r=3}^{\infty} \sum_{t_f \in F_r} h^{r-1} c(t_f) H(t_f)(y), \tag{5.7}$$

Table 5.2: 2-loop equations from topologically non-equivalent K-loops, from order 2 to order 5.

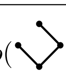
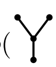
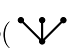
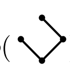
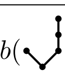
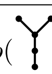
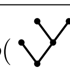
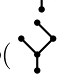
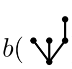
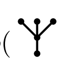
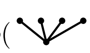
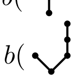
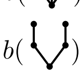
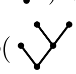
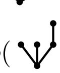
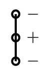
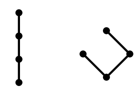
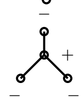
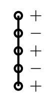
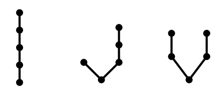
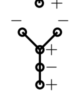
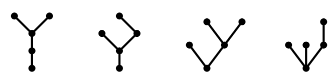
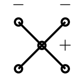
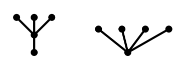
Order	2-loop equations
2	$b($  $) = 0$
3	$b($  $) + b($  $) = 0$
4	$b($  $) + b($  $) = 0$ $b($  $) + b($  $) = 0$ $b($  $) = 0$
5	$b($  $) + b($  $) = 0$ $b($  $) + b($  $) = 0$ $b($  $) + b($  $) = 0$ $b($  $) + b($  $) = 0$ $b($  $) + b($  $) = 0$ $b($  $) + b($  $) = 0$

Table 5.3: Free trees (vertices denoted by circles) and their associated rooted trees (vertices denoted by discs) from order 1 to 5. Superfluous free trees are without ±.

$r(t)$	Free tree $t_f \in F$	Rooted trees $t \in T$
1		
2		
3		
4		
4		
5		
5		
5		

where $c : T \mapsto \mathbb{R}$ are the coefficients associated with free trees t_f. Note that for order 1, $c(\circ) = 1$.

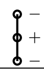
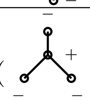
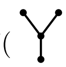
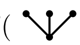
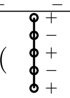
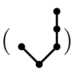
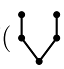
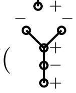
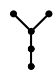
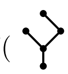
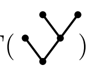
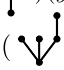
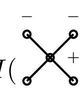
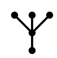
For volume preservation, the divergence-free condition must be applied to (5.7), forming K-loops from the rooted trees as in Section 5.1. By the linear independence and topological equivalence of K-loops, similarly to Section 5.1, a system of linear equations for each order can be extracted, and it can be concluded that only trivial coefficients can satisfy the divergence-free condition. However, this technique restricts the calculation to a finite order. To overcome this restriction, the discussion below presents another proof which shows that all coefficients in (5.7) must be trivial for all orders if the B-series method is to preserve volume exactly.

Before this proof is presented, several issues related to free trees $t_f \in F$ need be discussed, and they are presented in the following propositions and lemma.

Definition 5.2. *A vertex of a free tree has* degree $s = m$ *if there are* m *edges incident with it.*

A tall *free tree is a free tree where each vertex has degree* $s \leq 2$.

Table 5.4: Hamiltonian combinations $H(t_f)(y)$ of elementary differentials for non-superfluous free trees from order 1 to 5.

$r(t)$	Hamiltonian vector field
1	$H(\circ_{+})(y) = F(\bullet)(y) = f(y)$
2	———
3	$H($  $)(y) = -F($ $)(y) + \frac{1}{2}F($  $)(y)$
4	$H($  $)(y) = -\frac{1}{2}F($  $)(y) + \frac{1}{3!}F($  $)(y)$
5	$H($  $)(y) = F($  $)(y) - F($  $)(y) + \frac{1}{2}F($  $)(y)$
5	$H($  $)(y) = \frac{1}{2}F($  $)(y) - F($  $)(y) - \frac{1}{2}F($  $)(y)$ $+ \frac{1}{2}F($  $)(y)$
5	$H($  $)(y) = -\frac{1}{3!}F($  $)(y) + \frac{1}{4!}F($  $)(y)$

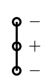
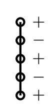
A vertex of degree $s \geq 3$ is called a junction.

A junction is called terminal *if it has at least two* tall *trees incident with it.*

Proposition 5.2. *Every free tree with a junction has at least one terminal junction.*

Proof. For a finite free tree with at least one junction we begin by picking an arbitrary junction. The proposition holds if this junction has at least two tall trees incident with it. Otherwise, this junction has at most one tall tree incident with it, and is incident with at least two other edges leading to another junction each. This process continues and the number of tall trees incident with each new junction can be examined. Eventually, because the free tree is finite and has no cycles, one arrives at a junction made up of at least two tall trees (which might be leaves of the free tree). Hence it is a terminal junction. □

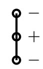
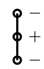
Proposition 5.3. *For order $r \geq 2$ the coefficient associated with the* tall *free tree of each order r is zero. That is,*

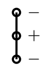
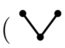
$c($  $) = c($  $) = c($  $) = c($  $) = \cdots = 0.$

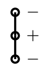
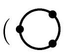
Proof. Recall that the coefficients b of *tall* rooted trees of order $r \geq 2$ appear in the modified differential equation in (5.1). For each order $r \geq 2$, the

r-loops are topologically non-equivalent to any other K-loops of the same order. By linear independence of K-loops and non-trivial evaluation of a source-free system, the associated tall tree coefficients b of order $r \geq 2$ must be zero. Since the modified differential equation (2.1) is equal to (5.7), coefficients c of the *tall* free trees of order $r \geq 2$ must also vanish. ☐

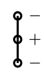
For example, the following modified differential equation up to order 3 can be constructed from (5.7).

$\widetilde{f}(y) = f(y) + h^2 c($  $)H($  $)(y) + O(h^3)$

$= f(y) + h^2 c($  $)\Big[-F($ $)(y) + \frac{1}{2}F($  $)(y)\Big] + O(h^3)$

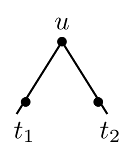
$\Longrightarrow \quad \nabla \cdot \widetilde{f}(y) = h^2 c($  $)\Big[-F($  $)(y)\Big] + O(h^3).$

Note that 2-loops are not present in the expansion since 2-loop equations vanish by virtue of Lemma 5.1. Then up to $O(h^3)$,

$\nabla \cdot \widetilde{f}(y) = 0 \quad \Longrightarrow \quad c($  $) = 0.$

Next, we present Lemma 5.4. This result allows us to reduce by one, the degree s (i.e. the number of incident edges) of any given terminal junction of a free tree.

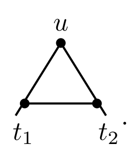
LEMMA 5.4. *Let $t_1, t_2 \in \{$tall trees in $T\} \cup \{\emptyset\}$ and u denote a forest of rooted trees in T. Then a recursion exists between the coefficient of the free tree containing t_1, t_2 and the forest u, and the coefficient associated with the free tree constructed by attaching a* tall *free tree in T to the root of forest u. That is,*

coefficient of  *is a multiple of* coefficient of  .

Note that "$\vdots$" indicates the possibility of multiple vertices, all of degrees $s = 2$. The forest u is grafted to the top vertex of the free trees in the relation, and this root of u is also terminal junction by Definition 5.2.

PROOF.

Consider a 3-loop of the form



The given 3-loop is produced by at most three distinct free trees, not counting symmetries. Such free trees can be recovered if each edge of the 3-loop is disconnected separately. Then by linear independence of K-loops, a homogenous linear relation can be stated between the coefficients of such free trees.

The Lemma is proved by induction on the sum of the number of vertices along the separate branches of t_1 and t_2, up to, but excluding, the terminal junction itself. Now, let

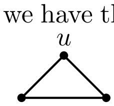
$$r_1 = r(t_1) + 1 \qquad \text{and} \qquad r_2 = r(t_2) + 1,$$

where $r_1 \geq 1$ (respectively, $r_2 \geq 1$) denote the order of the tree t_1 (respectively, t_2) and the vertex connecting the tall tree with the 3-loop. Define

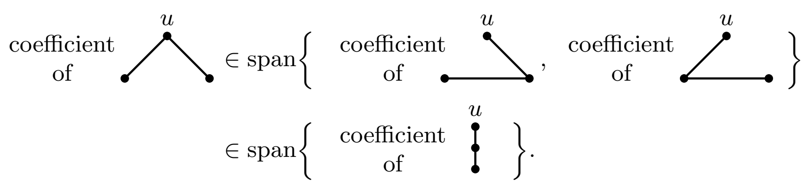
$$v = r_1 + r_2.$$

Since both t_1 and t_2 can be the empty tree $\emptyset$, $\min(v) = 2$. The proof is then given by induction on v.

- For $v = 2$, this implies $t_1 = t_2 = \emptyset$ and $r_1 = r_2 = 1$. When the divergence-free condition is applied to the corresponding 3-loop, we have the following

  linear combination of free trees coefficients for  $= 0$.

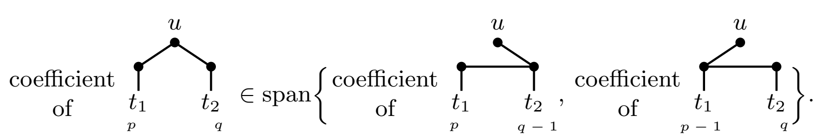
  The possible free trees can be identified, and this yields



  Hence the lemma holds for $v = 2$.

- To prove the lemma for all free trees with $r_1 \geq 1$ and $r_2 \geq 1$ we use induction on v. Note that in the following if $r_1 = 0$ then the branch attached to t_1 disappears, resulting in a single *tall* tree connected to the root of forest u. Similarly this is true when $r_2 = 0$.

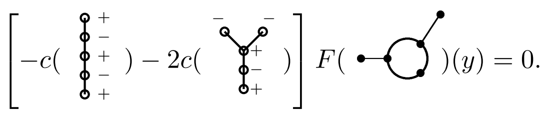
  Assume that the lemma holds for $v = r_1 + r_2 = N \geq 2$. Then, given $p + q = N + 1$, for a free tree with $r_1 = p$ and $r_2 = q$ we have



  Note that for each of the free trees in the span on the right hand side, the terminal junction has shifted along one, from the root of forest u to either the left or right vertex connecting t_1 or t_2. That is, the terminal junction of the first tree is the vertex connecting t_2 to the root of u, so $r_1 = p$, $r_2 = q - 1$ and $v = p + q - 1 = N$. Similarly the terminal junction of the second tree is now the vertex connecting t_1 to the root of u, so $r_1 = p$, $r_2 = q$ and $v = p + q - 1 = N$. By the induction hypothesis the lemma is true for $v = N$,and this implies that it is true also for $v = N+1$. Therefore, Lemma 5.4 holds for all $v \geq 2$ such that $r_1 \geq 1, r_2 \geq 1$.

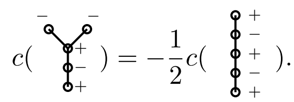
□

Note that this result is referred to as *edge reduction of a terminal junction*, since the relation in Lemma 5.4 yields free trees in the span, where for each free tree the degree s of the root of u is reduced by one. For example, one of the $O(h^4)$ terms in $\nabla \cdot \widetilde{f}(y) = 0$ involving a contracted elementary differential of order 5 is

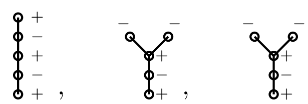


For a general volume-preserving differential equation this implies

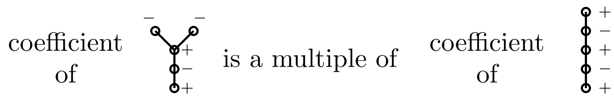
(5.8)



To recover this linear dependence by Lemma 5.4, it is observed that the 3-loop can be represented if u and t_1 are order-1 rooted trees, and $t_2 = \emptyset$. Disconnecting each edge of the 3-loop separately, the following free trees of order 5 are recovered,



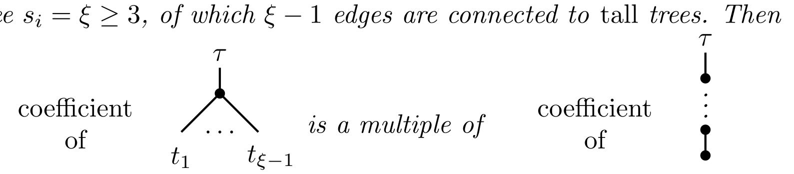
Hence,



and the linear dependence expressed in (5.8) is recovered.

It is important to note that we can apply Lemma 5.4 to an *arbitrary* terminal junction at any position of a free tree of order $r \geq 4$. This allows us to consider the situation in Lemma 5.5, which removes a particular type of terminal junction from a free tree, thereby reducing the total number of terminal junctions of the free tree by one.

Lemma 5.5. *Consider a free tree of order $r \geq 4$ with a terminal junction of degree $s_i = \xi \geq 3$, of which $\xi - 1$ edges are connected to* tall *trees. Then*



where $\{t_1, \ldots, t_{\xi-1}\}$ are tall trees in T of order $r \geq 1$, and τ is a rooted tree of order $r \geq 1$ such that the root of τ is attached to the terminal junction i.

Proof.

Proceeds at once by repeated application of lemma 5.4. □

We refer to Lemma 5.5 as the *reduction of terminal junctions* of a free tree, since it is clear that for a free tree with terminal junction i of degree $s_i = \xi$, the tall trees $\{t_1, \ldots, t_{\xi-1}\}$ attached to terminal i are effectively merged into a *single* tall tree by the relation in the lemma. Hence the vertex i is no longer a terminal junction and so the total number of terminal junctions in the free tree is reduced by one. This consequence of Lemma 5.5 is important in the proof of Theorem 5.6.

THEOREM 5.6. *Let a volume-preserving differential equation be denoted by* $\dot{y} = f(y)$. *For order* $r \geq 2$, *the coefficient* $c(t_f)$ *of each free tree* $t_f \in F$ *in the modified vector field* (5.7) *of a volume-preserving* B*-series method, must be zero. That is*

$$\widetilde{f}(y) = f(y).$$

The proof of this theorem consists of two parts: in the first part we prove that the coefficient $c(t_f)$ of any free tree of order $r(t_f) \geq 2$ is recursively related to the coefficient of the *tall* free tree of the same order; and in the second part we show that all coefficients $c(t_f)$ in (5.7) must be trivial, apart from the coefficient of the order-1 free tree.

In the discussion below, free trees are studied according to the number of terminal junctions they contain, rather than by their order. Classifying them in this manner covers all free trees of order $r \geq 2$, apart from the tall free trees.

PROOF. **Part One: There exists a recursion between the coefficient of any free tree of order $r \geq 2$ and the coefficient of the tall free tree of the same order.**

It is clear that Part One holds for free trees of order two and order three, since there exist no free trees at these values which are not *tall* free trees .

Beginning the proof for free trees of order $r \geq 4$, it is important to note that all free trees which are not tall free trees must contain at least one terminal junction (by Proposition 5.2), which is of degree $s = \xi$ (where $s \geq 3$), such that $\xi - 1$ incident edges are attached to *tall* trees of order $r \geq 1$. This is obvious for a free tree with one or two terminal junctions. For a free tree with more than two terminal junctions, suppose that we start from a terminal junction connected to at least two other terminal junctions of the free tree, and move along branches of the free tree to the next terminal junction. Since the number of vertices of the free tree is finite, then, moving from one terminal junction to another terminal junction, we eventually shall trace an edge in the free tree that leads to a terminal junction where its remaining edges are connected to no other terminal junctions. That is, its remaining edges are connected (eventually) to *leaves* of the free tree. Such a terminal junction must be of degree $s = \xi$ where $\xi - 1$ edges are connected to tall trees.

Hence, Lemma 5.5 can be applied repeatedly to any (finite) free trees which are not tall trees, such that by recursion, the number of terminal junctions of the free tree eventually reduces to zero (i.e. a tall tree). This yields the desired result for Part One.

Part Two: If the modified differential equation $\dot{y} = \widetilde{f}(y)$ for a *B*-series method is to satisfy the volume-preserving condition then the coefficients $c(t_f)$ for all free trees of orders $r(t_f) \geq 2$ in (5.7) are zero.

By Proposition 5.3, all *tall* free tree coefficients (both superfluous and non-superfluous), are trivial. Since Part One establishes a recursion between any coefficients of free trees and the coefficients of tall free trees, *all* coefficients for $r(t_f) \geq 2$ must be zero.

This completes the proof of Theorem 5.6.

□

*5.4 Consequence of Theorem 5.6 for general volume-preserving **B**-series methods*

Recall that Theorem 5.6 states that all coefficients $c(t_f)$ in (5.7) must be trivial if a B-series method is to integrate a general source-free differential equation whilst preserving volume. This means that the modified differential equation must be exactly the same as the original differential equation,

$$\dot{y} = \widetilde{f}(y) = f(y).$$

Note that this requirement is impossible to satisfy in general because it implies that the B-series method should have truncation errors smaller than any power of h, and in the general case, the exact solution y of a volume-preserving system $\dot{y} = f(y)$ is not known. This is summarised in the following theorem, which is the main result of this paper.

THEOREM 5.7. *B-series methods cannot preserve volume directly for a general volume-preserving differential equation*[2]*.*

Since B-series methods are the main methods that preserve all linear symmetries of ODEs, the above result also sheds further doubt on the existence of integrators that simultaneously preserve volume and all linear symmetries [12].

It is perhaps important to reiterate that Theorem 5.7 applies to a *general* source-free differential equation. There are in fact source-free systems with special structure for which volume-preserving B-series methods can be constructed. Examples of such systems can be found in [3].

6 Conclusion

This article presents a proof that B-series methods cannot preserve volume for general source-free differential equations in more than two dimensions, by applying the divergence-free condition to the modified differential equation of a volume-preserving B-series method. The divergence operator leads to the construction of the contracted elementary differentials and their graphical representations, the K-loops. By studying the relations between K-loops and their rooted (and free) trees, it is concluded that it is not possible to construct a volume-preserving geometric integrator by B-series methods.

[2] A picky reader might argue that this result is not correct, since the exact solution is a B-series. Our response to this would be that the exact solution is not a numerical *method*, i.e. it is not given for arbitrary vector fields.

Acknowledgements

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