Norwegian University
of Life Sciences

Master's Thesis 2023 30 ECTS
Faculty of the Science and Technology
Department of Mathematics

A study of volume-preserving methods with aromatic B-series

Mahmoud Naesan Menla Ali

Preface

This master's thesis represents the end of my five-year graduate studies in natural science with teacher education in science (LUR), at the Norwegian University of Life Sciences (NMBU). This thesis represents the studying of volume-preserving methods by using aromatic Butcher series. This work allowed me to immerse myself in mathematics. I hope that this work contribute in the next researches in this field.
I would like to express my gratitude to my thesis supervisors, Geir Bogfjellmo as the main supervisor from (NMBU), and the external supervisor Adrien Ange André Laurent from the University of Bergen for their invaluable guidance, support, and patience before and throughout my research. I would like to thank Hans Zanna Munthe-Kaas for his motivation, and the course about numerical methods and Butcher series. I would also like to thank the faculty members of Faculty of the Science and Technology for their help throughout my study.
Finally, I am grateful to my wife, Shahnaz, and our children, Sibar, Lewend, and Zahida for their love, patience, and support throughout this work.

Fredrikstad, May 2023

Mahmoud Naesan Menla Ali

Introduction

Since the difficulty and even impossibility of solving equations by traditional methods, the numerical methods play an essential role in understanding the dynamic behavior of a system and in solving physical and engineering problems [11]. The Taylor series, as a way of studying integrators of ordinary differential equations, have important properties. An most important example of these tools is the Butcher series or B-series. These were originally introduced by Butcher [3] and formulated by Hairer and Wanner [7] as a tool to study Runge–Kutta methods for the numerical solution of ordinary differential equations. The concept “B-series”, also known as the “Butcher series”, was introduced by Ernst Hairer and Gerhard Wanner in 1974. Each term in a Butcher series consists of a weighted elementary differential, and the set of all such differentials is isomorphic to the set of rooted trees. The significance of trees in mathematics was pointed out by Arthur Cayley (1857) [4]. Aromas and aromatic trees were invented by Iserles, Quispel, and Tse [10], and by Chartier and Murua [5]. A generalization of B-series is formed by the aromatic B-series introduced by Munthe-Kaas and Verdier. Aromatic B-series were a tool for the study of volume-preserving integrators, and they allow to compute the divergence of a B-series. Volume preservation as a geometric property can be encountered in a large class of dynamical systems with many applications, for instace, it underlies ergodic theory and thus statistical mechanics, and it appears in the tracking of particles in incompressible fluid flow [10]. As we know, the Runge-Kutta methods can not preserve volume for all linear source-free ODEs [10]. It has been proved by Feng and Shang. The exponential Runge–Kutta (ERK) methods do preserve volume for all linear source-free ODEs [10]. ERK methods cannot preserve volume for all nonlinear ODEs. It has been proved by Iserles, Quispel, and Tse [10], and also by Chartier and Murua [5]. B-series methods (which include RK, ERK, and several more classes of methods) cannot preserve volume for all source-free ODEs. But the aromatic B-series do. We are interested in finding the conditions of the volume-preserving by using the aromatic B-series. The structure of this thesis is as follows: in the first chapter, we introduce the background on the numerical integration methods, Taylor series, B-series, and aromatic B-series with more details. We introduce structures of aromas and elementary differential. In the second chapter, we introduce the divergence as an operator and the condition of volume-preserving methods. The important part of Chapter 2 is using aromatic B-series as a numerical integration. The last part is the Appendices which include more details of the computations that occurred in Chapter 2. All computations in Chapter 2 are up to order 2 or 3, but in the appendices, computations are presented up to order 5.

Contents

Chapter 1

Series and Numerical Methods

Series have been a tool for studying numerical integrators of ODEs. Taylor and Taylor's expansion is used for representing a function as an infinite sum of terms. Taylor expansion uses for function approximation with finite terms. The Butcher series or B-series, are introduced by Butcher and by Hairer and Wanner [1], as a tool to study Runge-Kutta methods for the numerical solution of ordinary differential equations.

1.1 Taylor series

Before beginning with the Butcher series, we recall the Taylor series and Taylor expansion [16].

Definition 1.1.1. *let f be a function with derivatives of all orders throughout some interval containing a as an interior point. Then the Taylor series generated by f at x=a is:*

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \cdots .$$

Or it can be written like this:

$$f(a+h) = f(a) + \frac{h}{1!}f'(a) + \frac{h^2}{2!}f''(a) + \cdots + \frac{h^n}{n!}f^{(n)}(a) + \cdots . \tag{1.1}$$

1.1.1 Differential equations

An ordinary differential equation is expressed in the form

$$\dot{x} = \frac{dx}{dt} = f(t, x(t)), \quad where \quad f : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N \tag{1.2}$$

or, written in terms of individual components,

$$\begin{aligned}
\frac{dx^1}{dt} &= f^1(t, x^1(t), x^2(t), ..., x^N(t)), \\
\frac{dx^2}{dt} &= f^2(t, x^1(t), x^2(t), ..., x^N(t)), \\
&\vdots \\
\frac{dx^N}{dt} &= f^N(t, x^1(t), x^2(t), ..., x^N(t)).
\end{aligned} \tag{1.3}$$

This can be formulated as an autonomous problem

$$\dot{x} = f(x(t)), \quad f : \mathbb{R}^N \to \mathbb{R}^N$$

by increasing N if necessary and introducing a new dependent variable x^0 which is forced to always equal x. The autonomous form of (1.3) becomes

$$\begin{aligned}
\frac{dx^0}{dt} &= 1, \\
\frac{dx^1}{dt} &= f^1(x^0(t), x^1(t), x^2(t), ..., x^N(t)), \\
\frac{dx^2}{dt} &= f^2(x^0(t), x^1(t), x^2(t), ..., x^N(t)), \\
&\vdots \\
\frac{dx^N}{dt} &= f^N(x^0(t), x^1(t), x^2(t), ..., x^N(t)).
\end{aligned}$$

1.2 B-Series

The Butcher series are mathematical objects introduced by the New Zealand mathematician John Butcher in the 1960s. He introduced them as part of his study of Runge–Kutta methods, a popular class of numerical methods for evolution equations such as initial-value problems for ordinary differential equations. They remain indispensable in the numerical analysis of differential equations [13]. Butcher series are intimately associated with the set of smooth (infinitely differentiable) vector fields on vector spaces. Indeed, let f be a smooth vector field on a vector space $\mathbb{R}^n$, defining the ordinary differential equation (ODE) (1.2). Let $x(h)$ be the solution of the differential equation (1.2) at time $t = h$, and the initial condition is $x(0) = x_0$. The solution $x(h)$ can written as a Taylor series:

$$x(h) = x(0) + h\dot{x}(0) + \frac{h^2}{2!}\ddot{x}(0) + \frac{h^3}{3!}\dddot{x}(0) + \cdots . \tag{1.4}$$

And the other terms can be written as follows after chain and product rules:

$$\begin{aligned}
\dot{x} &= f(x), \\
\ddot{x} &= \frac{d}{dt}\dot{x} = \frac{d}{dt}f(x) = f'(x)\dot{x} = f'(x)f(x), \\
\dddot{x} &= f'(x)f'(x)f(x) + f''(x)(f(x), f(x)), \\
x^{(4)} &= f'(x)f'(x)f'(x)f(x) + f'(x)f''(x)(f(x), f(x)) + 3f''(x)(f'(x)f(x), f(x)) + f'''(x)(f(x), f(x), f(x)), \\
&\vdots
\end{aligned}$$

If we substitute f and its derivatives in the Taylor series (1.4), we find the form:

$$x(h) = x(0) + hf + \frac{h^2}{2}f'f + \frac{h^3}{6}f'f'f + \frac{h^3}{6}f''(f, f) + \cdots . \tag{1.5}$$

Where f and its derivatives are called an *elementary differentials*, and where each elementary differential is evaluated at x_0. Notice that the power of h in each term is determined by the multiplicity of f in the elementary differential. However, the coefficients 1, 1, 1/2, 1/6, 1/6, and so on are not determined by their corresponding elementary differentials. A Butcher series, shortly denoted B-series, is a generalization of allowing arbitrary coefficients, i.e., a formal series of the form:

$$B(c, f) := c_0 x(0) + c_1 h f + c_2 h^2 f' f + c_3 h^3 f' f' f + c_4 h^3 f''(f, f) + \cdots . \tag{1.6}$$

where $c_i \in \mathbb{R}$.

1.2.1 Rooted Trees

Here we will explain the context for the given autonomous problem:

$$\begin{aligned} \dot{x} = f(x(t)); \quad & x(t_0) = x_0, \\ & x : \mathbb{R} \to \mathbb{R}^N, \\ & f : \mathbb{R}^N \to \mathbb{R}^N \end{aligned}$$

written in component form:

$$\frac{dx^i}{dt} = f^i(x^1, x^2, ..., x^N), \quad where \quad i = 1, 2, ..., N$$

The second derivative of x^i can be obtained by the chain rule followed by substitution of the known first derivative of a generic component f^i. That is,

$$\frac{d^2 x^i}{dt^2} = \sum_{j=1}^{N} \frac{\partial f^i}{\partial x_j} \frac{\partial x^j}{\partial t} = \sum_{j=1}^{N} \frac{\partial f^i}{\partial x_j} f^j. \tag{1.7}$$

This can be written in a more compact form by using subscripts to indicate partial x derivatives. That is,

$$f^i_j = \frac{\partial f^i}{\partial x^j}.$$

A further simplification results by adopting the "Einstein summation convention", in which repeated suffixes in expressions like $f^i_j f^j$, imply summation without this being written explicitly. Hence, we can write:

$$\frac{d^2 x^i}{dt^2} = f^i_j f^j.$$

We take this further and find formulae for the third and fourth derivatives:

$$\begin{aligned} \frac{d^3 x^i}{dt^3} &= f^i_{jk} f^j f^k + f^i_j f^j_k f^k, \\ \frac{d^4 x^i}{dt^4} &= f^i_{jkl} f^j f^k f^l + 3 f^i_{jk} f^j f^k_l f^l + f^i_j f^j_{kl} f^k f^l + f^i_j f^j_k f^k_l f^l, \\ &\vdots \end{aligned} \tag{1.8}$$

And simple writing, we "disregard" the use of indexes (i, j, k, ...), then we get the form:

$$\begin{aligned} \frac{dx}{dt} &= f, \\ \frac{d^2 x}{dt^2} &= f' f, \\ \frac{d^3 x}{dt^3} &= f''(f, f) + f' f' f, \\ \frac{d^4 x}{dt^4} &= f'''(f, f, f) + 3 f''(f' f, f) + f' f''(f, f) + f' f' f' f, \\ &\vdots \end{aligned} \tag{1.9}$$

Thus, the Taylor series:

$$x(t_0+h) = x_0 + hf + \frac{h^2}{2}f'f + \frac{h^3}{6}f'f'f + \frac{h^3}{6}f''(f,f) + \cdots . \tag{1.10}$$

1.2.2 Graphs and trees

A directed graph in mathematics is a set of vertices and a set of edges between some of the ordered pairs of vertices. It is convenient to name or label each of the vertices and use their names in specifying the edges. If V is the set of vertices and E is the set of edges, then the graph is referred to as (V, E) [4].
Basic terminology and observations:

1. A graph is connected if between any pair of vertices, the sequence of vertices such that any successive pair is connected by an edge (we ignore the direction).
2. A loop is a sequence of vertices where the first and the last vertex is the same, and each vertex is joined by an edge respectively.
3. The order of a graph is the number of vertices.
4. A tree is a connected graph with at least one vertex and with no loops.
5. For a tree, the number of edges is one less than the number of vertices. (that means n vertices, $n-1$ edges)
6. The "empty tree" $\emptyset$, with V = E = $\emptyset$, is sometimes included, as an additional tree.
7. The set of trees with a positive number of vertices will be denoted by $\mathcal{T}$ and the set of trees, with $\emptyset$ included by $\mathcal{T} \cup \{\emptyset\}$.

1.2.3 The importance of studying trees

There is a good reason for studying trees, both rooted and unrooted. Trees play a central role in the formulation of order conditions for Runge-Kutta and other numerical methods. In particular, elementary differentials, which are building blocks of B-series and aromatic B-series, are indexed on the set of rooted trees. Furthermore, unrooted trees emerge as fundamental concepts in the theory of symplectic methods and their generalizations [4, 7]. Examples of trees are shown in the table (1.1).

Definition 1.2.1 (Order of a tree [4]). *The order of the tree τ = (V, E) is $|\tau| = |V|$.*

Definition 1.2.2 (Symmetry of a tree). *The symmetry of a tree τ, written $\sigma(\tau)$, is the order of the group $A(\tau)$, where $A(\tau)$ is the group of automorphism of τ.*

Theorem 1.2.1 (Symmetry coefficients) $\sigma(\tau)$). *The symmetry coefficients $\sigma(\tau)$ are defined by:*
$\sigma(\bullet) = 1$ and,
$\sigma(\tau) = \Pi_{i=1}^{m} k_i!\sigma(\tau_i)^{k_i}, \quad for \quad \tau = [\tau_1^{k_1}\tau_2^{k_2}...\tau_m^{k_m}]$

Definition 1.2.3 (Elementary Differentials). *For a tree $\tau \in \mathcal{F}$ the elementary differential is a mapping $\mathcal{F}(\tau) : \mathbb{R}^n \to \mathbb{R}^n$, defined recursively by $\mathcal{F}(\bullet)(x) = f(x)$ and*

$$\mathcal{F}(\tau)(x) = f^{(m)}(x)(\mathcal{F}(\tau_1)(x), \cdots, \mathcal{F}(\tau_m)(x)),$$

for $\tau = [\tau_1, \cdots, \tau_m]$

The quantities $|\tau|$, $\sigma(\tau)$ and $\mathcal{F}(\tau)$ for all trees up to order 4 are given in Table 1.1 See the table (1.1)

1.2.4 The relation between elementary differential and rooted trees

John Butcher explains clearly the structure of the elementary differentials, and crucially, shows how they are in one-to-one correspondence to rooted trees. This development, perhaps regarded initially as a bookkeeping device for finding and keeping track of the different terms, has over time become central to the combinatorial and algebraic study of B-series. The expressions $f, f'f, f'f'f, f''(f,f), ...$ are examples of elementary differentials, and each of them corresponds to a graph like a tree. To explain the relation between a graph and the corresponding elementary differential, we will call f a child or grandchild, and $f', f'', f''', ...$ a parent or grandparent. It depends on the form of the graph. The tree that corresponds to f' is a node with a link to a possible child (f). The term $f'f$ corresponds to this link having been made to the child represented by$f$. The term f'' corresponds to a node with two possible links, but in $f''(f,f)$ these links are filled with copies of the child represented by f. Finally, the term $f'f'f$ corresponds to a three-generation family with the first f' playing the role of grandparent, the second f' playing the role of a parent, and the final operand f playing the role of grandchild and child, respectively, of the preceding f' operators [4]. The rooted trees $(\mathcal{T})$, and their associated elementary differentials $\mathcal{F}(\mathcal{T})$ are shown in the table (1.1). $\sigma(\tau)$ denotes the symmetry of the rooted trees. See the table below (1.1).

Order	Tree(τ)	symmetry σ	$\mathcal{F}(\tau)$
0	$\emptyset$	1	x
1		1	f
2		1	$f'f$
3		1	$f'f'f$
		2	$f''(f,f)$
4		1	$f'f'f'f$
		1	$f''(f'f,f)$
		2	$f'(f''(f,f))$
		6	$f'''(f,f,f)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Table 1.1: The relation between trees, elementary differentials, and their symmetries

1.2.5 B-Series

B-series are a formalism for expressing the Taylor series for the solution to questions written in terms of the triple (x, h, f). They are always written in terms of elementary differentials, which in turn are indexed by the trees [4].

Definition 1.2.4. *Let a is a mapping a: $\mathcal{T} \cup \{\emptyset\} \to \mathbb{R}$, where $a(\emptyset) = 1$. Then the B-series is a formal series defined by:*

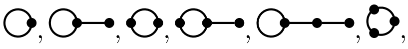
$$(\beta_f a)x = a(\emptyset)x + \sum_{\tau \in \mathcal{T}} \frac{h^{|\tau|}a(\tau)}{\sigma(\tau)} \mathcal{F}_f(\tau)(x), \tag{1.11}$$

where τ is a tree, $\mathcal{T}$ is the set of trees, $|\tau|$ is the order of a tree. $\sigma(\tau)$ is the symmetry of τ, and $\mathcal{F}_f(\tau)$ is the mapping of the elementary differentials.

1.3 Aromatic B-series

1.3.1 Aromas

Definition 1.3.1 (Aromas)**.** *An aroma is a connected directed graph where each vertex has exactly one outgoing edge.*

It can be shown that an aroma has to contain exactly one cycle [2]. The smallest aromas are:  $, \cdots$. To simplify graphics, directions of edges are not shown unless they are necessary to distinguish between aromas. The edges are oriented so that the ring is a cycle and other edges are oriented towards the ring. Aromas and aromatic trees were originally introduced by Iserles, Quispel, and Tse [10], and by Chartier and Murua [5]. While generalization of B-series is formed by the aromatic B-series, introduced by Munthe-Kaas and Verdier, and their structure was investigated by Munthe-Kaas and Verdier [14] and by Bogfjellmo [1]. We will refer to the set of aromas as $\mathcal{A}'$ and the set of multisets (products) of aromas as $\mathcal{A}$. The empty multiset will be denoted by 1. Given a vector field f, an aroma λ represents a scalar function $\mathcal{F}(\lambda)$ according to the following procedure:

1- Label each node i, j, k, $\cdots$

2- For each node with label i, form the factor $f^i_{j_1,j_2,\ldots,j_m}$ where $j_1, j_2, ..., j_m$ are the labels of the nodes pointing towards node i. The upper index on f corresponds to vector components, and the lower to partial derivatives with respect to coordinate directions, i.e.

$$f^i_{j_1 j_2 \cdots j_m} = \frac{\partial^m f^i}{\partial x_{j_1} \partial x_{j_2} \cdots \partial x_{j_m}}. \tag{1.12}$$

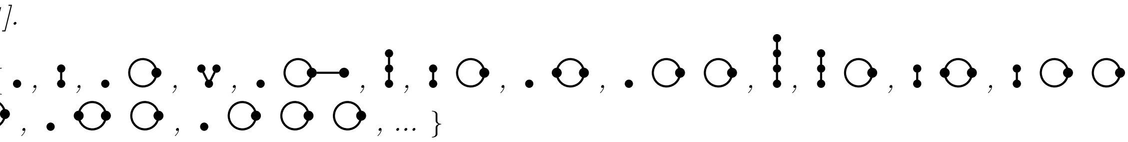
3- Finally, take the product of the factors and sum all terms using Einstein's summation convention.

1.3.2 Details about aromas

Definition 1.3.2 (Directed graphs)**.** *A directed graph $\gamma = (V, E)$ is defined by a finite set of vertices, and a set of edges $E \subseteq V \times V$. We say that the edge (v_1, v_2) goes out of v_1 and into v_2. A subgraph of γ, is another directed graph (W, F) where $W \subseteq V$, and $F \subseteq W \times W \cap E$.*
In this definition of graph, we allow the empty graph with 0 vertices and self-loops [1].

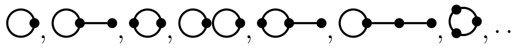
Definition 1.3.3 (Directed predecessor)**.** *On a given graph, we define the direct predecessor function π_γ from V to the power set of V by $v_1 \in \pi_\gamma(v_2)$ iff $(v_1, v_2) \in E$.*

Definition 1.3.4 (Aromatic forest)**.** *An aromatic forest is an equivalence class of directed graphs where each node has at most one outgoing edge. We denote the set of aromatic forests as $\mathcal{A}\mathbf{F}$. A root of an aromatic forest is a node with zero outgoing edges. The set of roots of the aromatic forest ϕ is denoted $r(\phi)$ [1].*

$\mathcal{A}\mathbf{F}$ ={  , ... }
where $\mathcal{A}\mathbf{F} = \mathcal{A} \times \mathbf{F}$

Result from the definition: An aromatic forest consists of connected components, each of which has either (i) one root, in which case the connected component is a *rooted tree*, or (ii) no roots, in which case it contains exactly one cycle and is called an *aroma*.

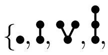
Definition 1.3.5 (Some subsets of aromatic forests)**.** *$\mathcal{A}$ is the set of aromatic forests with no roots.*

$\mathcal{A} = \{1,$  $, \cdots\}.$

$\mathcal{A}'$ is the set of connected aromatic forests with no roots, or aromas.

$\mathcal{A}' = \{$  $, \cdots\}.$

$\mathcal{T}$ is the set of rooted trees, or connected aromatic forests with exactly one root.

$\mathcal{T} = \{$  $, \cdots\}.$

$\mathcal{AT}$ is the set of aromatic forests with exactly one root. Where $\mathcal{AT} = \mathcal{A} \times \mathcal{T}$ (Cartesian product)

$\mathcal{AT} = \{$  $, \cdots\}.$

1.3.3 Geometric properties of aromatic B-series

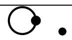
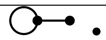
A fundamental property of the exponential map [1] is its equivariance with respect to the full group of diffeomorphisms on the domain. This means that if a vector field is transformed by a diffeomorphism and afterward exponentiated, we obtain exactly the same result as if the original vector field is exponentiated and the result is transformed by given diffeomorphism [4]. B-series methods have the property that this modified vector field $\tilde{f}$ can be expanded in a specific form:

$$\tilde{f} = b_0 f + b_1 f'(f) + b_2 f''(f, f) + b_3 f'(f'(f)) + \cdots . \tag{1.13}$$

where the terms are indexed by rooted trees. The first few terms of the expansion of a local, affine equivariant method, are of the form:

$$\phi(f) = b_0 f + b_1 f'(f) + b_2 div(f) f + b_3 f''(f, f) + b_4 \langle grad(div(f)), f\rangle f + \cdots . \tag{1.14}$$

By comparing (1.13) and (1.14), we observe that terms of a new kind appear, such as $grad\langle div(f)\rangle f$. We are able to completely describe those terms, and they turn out to be associated with *aromatic trees*, which are generalized rooted trees. The aromatic trees corresponding to the terms in (1.14) are the following, where the new terms are emphasized [14]:

Tree or aroma	Elementary differential
	f
	$f'f$
	$div(f)f$
	$f''(f,f)$
	$\langle grad(div(f)), f\rangle f$
$\vdots$	$\vdots$

1.3.4 Elementary differentials on aromas

A given vector field f, to any aromatic forest γ, there corresponds an elementary differentials $\mathcal{F}(\gamma)$. The quantity $f^i_{j_1 j_2 \cdots j_n}$ shows that that the upper index on f corresponds to the vector components and the lower indexes are partial derivatives with respect to the coordinate directions,

$$f^i_{j_1 j_2 \cdots j_n} = \frac{\partial^n f^i}{\partial x_{j_1} x_{j_2} \cdots \partial x_{j_n}}. \tag{1.15}$$

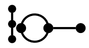
For example, an elementary differential is the following tree, with three nodes and two edges:

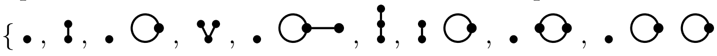
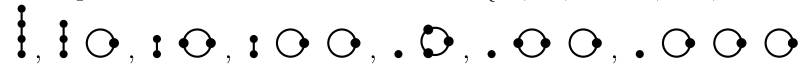
$$\gamma = \text{ } \tag{1.16}$$

$$\longrightarrow \mathcal{F}(\gamma) = f^i_{jk} f^j f^k.$$

[1] exp is defined by the property that: $u'(x) = f(x)$ and $u(0) = x_0$.

where $\mathcal{F}_f$ is the bijective function from $\mathcal{T}$ to the set of elementary differentials formed from f [1]. And an example of an aromatic forest that contains a tree and an aroma:

$\gamma =$  $\longrightarrow \mathcal{F}(\gamma) = f^i_j f^j_k f^k f^l_{mn} f^m_l f^n.$

NB: We have to know that often, when we draw a graph without orientation, that means that it is oriented in the counterclockwise direction. And the root of a tree is the bottom node, and the direction of the edges goes towards the root [14]. We provide a set with aromatic trees of orders up to 4. This set will help us to find the traces later. $\mathcal{AF}$ ={   , ... }.

Munthe-Kaas and Verdier showed that a larger class of methods, *Aromatic B-series methods*, are equivariant under all invertible affine maps [1]. The crucial difference between B-series and aromatic B-series is that in the aromatic case, *trace operations* are also allowed in forming elementary differentials, e.g. $Tr(f')f = (divf)f$ (see [6]). These elementary differentials are obtained by replacing the set of rooted trees with a larger set of directed graphs [1], e.g.

$Tr(f')f = \mathcal{F}_f($  $)$

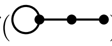
This property is very important to use aromatic B-series inside the Newton-Girard formula (2.4), which we will use it to obtain the volume-preserving method.

Examples: Some examples of elementary differentials:

$\mathcal{F}(1) = 1,$

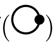
$\mathcal{F}($  $) = \sum_i f^i_i$

$\mathcal{F}($  $) = \sum_i f^i_j f^j_i$ (1.17)

$\mathcal{F}($  $) = \sum_i f^i_{ij} f^j_k f^k$

$\vdots$

The simplest aromas are the cyclic aromas,  , ... whose images under $\mathcal{F}$ are traces of powers of f'

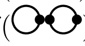
$\mathcal{F}($  $) = Tr(f') = div(f),$

$\mathcal{F}($  $) = Tr(f'^2),$

$\mathcal{F}($  $) = Tr(f'^3),$ (1.18)

$\mathcal{F}($  $) = Tr(f'^4),$

$\vdots$

Explanation: As Bogfjellmo explain in [1], when ϕ contains no aromas, the elementary differential operator $\mathcal{F}_f(\phi)$ corresponds to the product of elementary differential operators. If $\gamma \in \mathcal{A}$, then $\mathcal{F}_f(\gamma)$ is a scalar field. If $\phi = \gamma\tau_1\tau_2\cdots\tau_n$, where $\gamma \in \mathcal{A}, \tau_i \in \mathcal{T}$, then $\mathcal{F}_f(\phi) = \mathcal{F}_f(\gamma)\mathcal{F}_f(\tau_1)\cdots\mathcal{F}_f(\tau_n)$ is the product of the scalar field $\mathcal{F}_f(\gamma)$ and n vector fields $\mathcal{F}_f(\tau_1), \mathcal{F}_f(\tau_2), \cdots, \mathcal{F}_f(\tau_n)$.
NB: The image of two aromas is a product of the images of everyone.
For example:
$\mathcal{F}($  $) = \mathcal{F}$  $)\mathcal{F}($  $) = Tr(f')^2,$
$\mathcal{F}($  $) = \mathcal{F}$  $)\mathcal{F}($  $) = Tr(f').Tr(f'^2).$

Definition 1.3.6 (Aromatic B-series)**.** *Let $a : \mathcal{AT} \cup \{\emptyset\} \to \mathbb{R}$, where $a(\emptyset) = 1$, and f be a smooth vector field on the finite-dimensional vector space W. The aromatic B-series of the coefficient map a is the following formal series*

$$(\beta_f a)x = a(\emptyset)x + \sum_{\tau \in \mathcal{AT}} \frac{h^{|\tau|}a(\tau)}{\sigma(\tau)} \mathcal{F}_f(\tau)x, \tag{1.19}$$

where $\sigma(\tau)$ is the size of the symmetry group of τ.

In [14] by Munthe-Kaas and Verdier, aromatic B-series methods are defined as integrators whose series expansions only contain terms of the form $\mathcal{F}_f(\tau)$, where τ is an aromatic tree. Munthe-Kaas and Verdier had earlier [14] showed that a larger class of methods, Aromatic Butcher series methods, are equivariant under all invertible affine maps.

Chapter 2

Volume Preservation with aromatic B-series Method

2.1 Divergence-free vector field

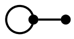
Divergence:
Divergence of a vector field: Let f be a vector field f: $\mathbb{R}^n \rightarrow \mathbb{R}^n$ then, the divergence of f is:

$$div(f) = \sum_i (\frac{\partial f^i}{\partial x_i}) = f_i^i \tag{2.1}$$

The main property of the aromatic B-series is to study volume-preserving integrators. There are many methods to study the existing volume-preserving integrators. Some methods are splitting methods and generating methods. And for the quadratic differential equation, there exists Kahan´s method (Hirota-Kimura method) discretization [8, 9] for the preservation of measures. A new methodology has been created by Laurent, McLachlan, and Munthe-Kaas [12] for the description of volume-preserving methods for solving general ordinary differential equations (1.2)
Divergence operator: The k-loops arise from acting the divergence operator on elementary differentials [10]. For instance, let we have the elementary differential of order 2 is $f_j^i f^j(y)$. If we apply the divergence on $f_j^i f^j(y)$ the divergence, this yields two separate contracted elementary differentials by the product rule, and they are represented by the 1-loop and the 2-loop, as it is shown below:
The divergence of elementary differentials $f_j^i f^j$ is

$$div(f_j^i f^j) = f_{ij}^i f^j + f_j^i f_i^j.$$

And by using trees and aromas, we find:

$div($  $) =$  $+$ .

The source-free dynamical systems on the Euclidean space $\mathbb{R}^n$ are defined by divergence-free vector fields $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$

$$div(f) = \sum_{i=1}^{n} \frac{\partial f^i}{\partial x_i} = 0. \tag{2.2}$$

One question raised by Munthe-Kaas and Verdier [14] is the existence of volume-preserving aromatic B-series methods. It is known that B-series methods cannot be volume-preserving (apart from the exact integrator), but that aromatic B-series methods can be [14]. However, it has so far not been possible to find an equation defining the update map for a volume-preserving aromatic B-series method [1]. Volume preservation is one of the qualitative characteristics common to many dynamical systems. Runge-Kutta methods can not preserve volume for all linear source-free ODEs. This has been proved by Feng and Shang. But Exponential Runge-Kutta methods can do preserve volume for all linear source-free ODEs (But not for all non-linear) [10]. In [10] Iserles, Quispel, and Tse proved that B-series methods (which include RK, ERK, and several more classes of methods) can not preserve volume for all source-free ODEs. Feng and Shang show that for a general (linear) source-free differential system of more than two dimensions, it is not possible to preserve volume by direct integration using classical methods(for example RK methods)

In fact, it is true that all divergence-free systems preserve volume in phase space [15].

Theorem 2.1.1. *(The Liouville´s theorem): Let $\dot{x} = f(x)$ be a system of ODEs on $\mathbb{R}^d$. Let $D \subset \mathbb{R}^d$ be open and bounded, let φ_t be the flow of f and set $D(t) = \varphi_t(D)$, and $v(t) = vol(D(t)) = \int_{D(t)} dV$. If $div(f) = 0$ then $v(t) = v(0)$ for all $t > 0$.*

Proof. Expanding the solution $y(t)$ with initial value $y(0) = y$ to the first order yields $x(t) = \varphi_t(x) = x + tf(x) + O(t^2)$. The formula for changing variables in multiple integrals gives:

$$v(t) = \int_{D(0)} det(\frac{\partial \varphi_t}{\partial x})dV.$$

Differentiating the expansion to the first order of $x(t)$ with respect to x we find

$$\frac{\partial \varphi_t}{\partial x} = I + \frac{\partial f}{\partial x}t + O(t^2), \quad for \quad t \to 0$$

For matrix A we have:

$$det(I + tA) = 1 + tTr(A) + O(t^2).$$

Consequently

$$det(\frac{\partial \varphi_t}{\partial x}) = det(I + \frac{\partial f}{\partial x}t + O(t^2)) = 1 + tTr(\frac{\partial f}{\partial x}) + O(t^2).$$

Since $Tr(\frac{\partial f}{\partial x}) = div(f)$, we get:

$$v(t) = \int_{D(t)} (1 + tdiv(f) + O(t^2))dV.$$

so at t=0

$$\frac{dv}{dt}|_{t=0} = \int_{D(0)} div(f)dV$$

The argument can be repeated for any $t_0 > 0$ and we simply get at t=0,

$$\frac{dv}{dt}|_{t=0} = \int_{D(t_0)} div(f)dV.$$

so for divergence free f we conclude that $\frac{dv}{dt} = 0$, and $v(t)$ is constant [15]. □

It is well known that intrinsic to all source-free systems, there is a volume form of the phase space $\mathbb{R}^n$, say

$$\alpha = dx_1 \wedge dx_2 \wedge ... \wedge dx_n, \tag{2.3}$$

such that the evolution of dynamics preserve this form. In other words, the phase flow φ_t, of source-free system $\dot{x} = f(x)$, satisfies the volume-preserving condition

$$\varphi_t^* \alpha = \alpha,$$

or equivalently,

$$det(\frac{\partial \varphi_t}{\partial x})(x) = 1.$$

for $x \in \mathbb{R}^n$ and $t \in \mathbb{R}$.

If $div(f) = 0$, the the solution of ODE is volume-preserving [12].
The flow of a differential equation $\dot{x} = f(x)$ in $\mathbb{R}^n$ is volume-preserving if and only if $divf(x) = 0$ for all x. For proof of this lemma, see [7].

2.2 Applying the Newton-Girard formula on Aromatic B-series

The Newton-Girard formula: The newton-Girard formula for symmetric polynomials from [2]:

$$det(I + hA) = P(r_1, ..., r_d), \tag{2.4}$$

where $r_i = Tr(h^i f'(x)^i)$ and P is a symmetric multivariate polynomial, each term of P is a trace of the order k. The first terms of (2.4) are:

$$det(I + hA) = 1 + hTr(A) + \frac{h^2}{2}(Tr(A)^2 - Tr(A^2)) + O(h^3).$$

We refer to (2.7) to see The Newton-Girard formula up to order 5.
Let us have the system of the ordinary differential equation (1.2)

$$\dot{x} = f(x)$$

An aromatic B-series method is a numerical integrator such that each individual step of the integrator can be expanded as an aromatic B-series:

$$x_{n+1} = x_n + \beta_f(a)(x_n). \tag{2.5}$$

where h is the step size and it is included in vector field f.
The first few terms of (2.5) are:

$$x_1^i = x_0^i + h\langle b, \bullet\rangle f^i + h^2\langle b, \rangle f^i_k f^k + h^2\langle b, \bullet\rangle f^k_k f^i + \cdots . \tag{2.6}$$

The terms up to order 5 are given in the appendix (A.1). We derive the equation (2.6) with respect to the component (j) [1]:

$$\frac{\partial x_1^i}{\partial x_0^j} = \delta^i_j + h\langle b, \bullet\rangle f^i_j + h^2\langle b, \rangle(f^i_{kj}f^k + f^i_k f^k_j) + h^2\langle b, \bullet\rangle(f^k_{kj}f^i + f^k_k f^i_j) + O(h^3).$$

We assume that $\langle b, \bullet\rangle = 1$, thus:

$$\frac{\partial x_1^i}{\partial x_0^j} = \delta^i_j + hf^i_j + h^2\langle b, \rangle(f^i_{kj}f^k + f^i_k f^k_j) + h^2\langle b, \bullet\rangle(f^k_{kj}f^i + f^k_k f^i_j) + O(h^3).$$

If we take h as a common factor, we find:

$$\frac{\partial x_1^i}{\partial x_0^j} = \delta^i_j + h(f^i_j + h\langle b, \rangle(f^i_{kj}f^k + f^i_k f^k_j) + h\langle b, \bullet\rangle(f^k_{kj}f^i + f^k_k f^i_j) + O(h^2)).$$

Now we write:

$$A^i_j = f^i_j + h\langle b, \rangle(f^i_{kj}f^k + f^i_k f^k_j) + h\langle b, \bullet\rangle(f^k_{kj}f^i + f^k_k f^i_j) + O(h^2).$$

[1]Some computations in the body of the thesis are only written up to order 2 or 3, but in the appendix, they are given up to order 5

Then,

$$\frac{\partial x_1^i}{\partial x_0^j} = \delta_j^i + hA_j^i.$$

By the Newton-Girard formula (2.4):

$$\begin{aligned} det(\frac{\partial x_1^i}{\partial x_0^j}) &= det(\delta_j^i + hA_j^i) \\ &= 1 + hTr(A) + \frac{h^2}{2}(Tr(A)^2 - Tr(A^2)) + \frac{h^3}{6}(Tr(A)^3 - 3Tr(A^2)Tr(A) + 2Tr(A^3)) \\ &+ \frac{h^4}{24}(Tr(A)^4 - 6Tr(A^2)Tr(A)^2 + 3Tr(A^2)^2 + 8Tr(A^3)Tr(A) - 6Tr(A^4)) \\ &+ \frac{h^5}{120}(Tr(A)^5 - 10Tr(A)^3Tr(A^2) + 20Tr(A^3)Tr(A)^2 + 15Tr(A)Tr(A^2)Tr(A^2) \\ &- 30Tr(A)Tr(A^4) - 20Tr(A^3)Tr(A^2) + 24Tr(A^5)) + O(h^6). \end{aligned} \tag{2.7}$$

Now we will try to find each term of (2.7) severally. Under the computations, we assume that $div(f) = 0$ because we study the volume-preserving. It means that all simple loops be zero under the map $\mathcal{F}$

$$\mathcal{F}(\ ) = \mathcal{F}(\ ) = \mathcal{F}(\ ) = \mathcal{F}(\ ) = 0.$$

A_j^i is given by the following (see (A.2) for the details).

$$\begin{aligned} A_j^i &= f_j^i + h\langle b, \ \rangle(f_{kj}^i f^k + f_k^i f_j^k) + h^2\langle b, \ \rangle(f_{kj}^i f_l^k f^l + f_k^i f_{lj}^k f^l + f_k^i f_l^k f_j^l) \\ &+ \frac{h^2}{2}\langle b, \ \rangle(f_{klj}^i f^k f^l + f_{kl}^i f_j^k f^l + f_{kl}^i f^k f_j^l) + \frac{h^2}{2}\langle b, \ \rangle(f_{lj}^k f_k^l f^i + f_l^k f_{kj}^l f^i + f_l^k f_k^l f_j^i) + O(h^3). \end{aligned}$$

Finding A_i^i: Here we will derive the equation (2.6) with respect to (i) and after that, we can find A_i^i we refer to (A.3)to see how it has been computed after that we vanish all simple loops from the set of aromatic forests.

$$\begin{aligned} A_i^i &= h\langle b, \ \rangle(f_j^i f_i^j) + h^2\langle b, \ \rangle(f_j^i f_{ki}^j f^k + f_j^i f_k^j f_i^k) \\ &+ \frac{h^2}{2}\langle b, \ \rangle(f_{jk}^i f_i^j f^k + f_{jk}^i f^j f_i^k +) + \frac{h^2}{2}\langle b, \ \rangle(f_{ki}^j f_j^k f^i + f_k^j f_{ji}^k f^i) + O(h^3). \end{aligned}$$

Now to simplify all these computations and indices writing, we will write (A.3) as aromatic functions:

$$A_i^i = h\langle b, \ \rangle(\ ) + h^2\langle b, \ \rangle(\ + \ ) + \frac{h^2}{2}\langle b, \ \rangle(2\ ) + \frac{h^2}{2}\langle b, \ \rangle(2\ ) + O(h^3).$$

See (A.4).

Now we can find the traces terms in (2.7) by using aromas

Tr(A):

$$Tr(A) = A_i^i = h\langle b, \ \rangle(\ ) + h^2\langle b, \ \rangle(\ + \ ) + \frac{h^2}{2}\langle b, \ \rangle(2\ ) + \frac{h^2}{2}\langle b, \ \rangle(2\ ) + O(h^3).$$

Tr$(A)^2$**:**

$$Tr(A)^2 = A_i^i A_j^j = h^2\langle b, \ \rangle^2(\ ) + O(h^3).$$

Tr(A^2)**:**

$$Tr(A^2) = A_t^i A_i^t = \ + h\langle b, \ \rangle(2\ + 2\ )$$

$$+ h^2 \langle b, \rangle (2 + 2 + 2) + \frac{h^2}{2} \langle b, \rangle (2 + 4)$$
$$+ \frac{h^2}{2} \langle b, \rangle (4 + 2) + h^2 \langle b, \rangle^2 (+ 2 +) + O(h^3).$$

Tr$(A)^3$

$$Tr(A)^3 = A^i_i A^j_j A^k_k = O(h^3).$$

Tr(A^2)**Tr(A)**

$$Tr(A^2)Tr(A) = h\langle b, \rangle ( ) + h^2 \langle b, \rangle^2 (2 + 2) + h^2 \langle b, \rangle (+)$$
$$+ \frac{h^2}{2} \langle b, \rangle (2) + \frac{h^2}{2} \langle b, \rangle (2) + O(h^3).$$

Tr(A^3)

$$Tr(A^3) = A^i_j A^j_s A^s_i = + h\langle b, \rangle (3 + 3)$$
$$+ h^2 \langle b, \rangle^2 (3 + 6 + 3) + h^2 \langle b, \rangle (3 + 3 + 3)$$
$$+ \frac{h^2}{2} \langle b, \rangle (3 + 6) + \frac{h^2}{2} \langle b, \rangle (6 + 3) + O(h^3).$$

Tr$(A)^4$**:**

$$Tr(A)^4 = O(h^4).$$

Tr(A^2)**Tr**$(A)^2$**:**

$$Tr(A^2)Tr(A)^2 = h^2 \langle b, \rangle^2 ( ) + O(h^3).$$

Tr(A^2**)**^{2}**:**

$$Tr(A^2)^2 = + h\langle b, \rangle (4 + 4) + O(h^2)$$

Tr(A^3**)Tr(A):**

$$Tr(A^3)Tr(A) = h\langle b, \rangle ( ) + O(h^2).$$

Tr(A^4)**:**

$$Tr(A^4) = A^i_j A^j_k A^k_l A^l_i = + h\langle b, \rangle (4 + 4) + O(h^2).$$

Tr$(A)^5$**:**

$$Tr(A)^5 = Tr(A)^4 Tr(A) = h^5 (\langle b, \rangle)^5 ( ) + O(h^6).$$

Tr$(A)^3$**Tr**(A^2)**:**

$$Tr(A)^3 Tr(A^2) = h^3 (\langle b, \rangle)^3 ( ) + O(h^4).$$

$\mathbf{Tr}(A^3)\mathbf{Tr}(A)^2$:

$$Tr(A^3)Tr(A)^2 = h^2\langle b, \rangle^2(\ ) + O(h^3).$$

$\mathbf{Tr}(A^3)\mathbf{Tr}(A^2)$:

$$Tr(A^3)Tr(A^2) = \ + O(h).$$

$\mathbf{Tr}(A)\mathbf{Tr}(A^2)\mathbf{Tr}(A^2)$:

$$Tr(A)Tr(A^2)Tr(A^2) = O(h).$$

$\mathbf{Tr}(\mathbf{A})\mathbf{Tr}(A^4)$:

$$Tr(A)Tr(A^4) = O(h).$$

$\mathbf{Tr}(A^5)$:

$$Tr(A^5) = A^i_j A^j_k A^k_l A^l_m A^m_i = \ + O(h).$$

2.3 Coefficients of the volume-preserving aromatic B-series method:

Now we substitute all traces which we have found in the formula (2.7), and collect all terms according to the aromatic function instead of the coefficients, we find the following:

$$\begin{aligned} det(I+hA) = 1 & \\ & + h^2\mathcal{F}(\ )(\langle b, \rangle - \frac{1}{2}) \\ & + h^3\mathcal{F}(\ )(\langle b, \rangle + \langle b, \rangle + \langle b, \rangle - \langle b, \rangle) \\ & + h^3\mathcal{F}(\ )(\langle b, \rangle - \langle b, \rangle + \frac{1}{3}) \\ & + O(h^4). \end{aligned}$$

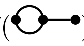
We refer to (A.23) for the more details of $det(I + hA)$. To find the conditions of the volume-preserving, we use the theorem (2.1.1). It means that $det(I+hA) = 1$. To obtain this condition, each term in (A.23) must equals zero. Consequently, the coefficient of each term equals zero as follows: the second term:

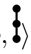
$$h^2(\langle b, \rangle - \frac{1}{2}) = 0 \Rightarrow \langle b, \rangle - \frac{1}{2} = 0 \Rightarrow \langle b, \rangle = \frac{1}{2}.$$

In the same way, we can find the value of the simple coefficients that correspond to the circle loops aroma (, , , , ...), as they are shown in the table below (2.1):

Coefficient	The value
$\langle b, \rangle$	$\frac{1}{2}$
$\langle b, \rangle$	$\frac{1}{6}$
$\langle b, \rangle$	$\frac{1}{24}$
$\langle b, \rangle$	$\frac{1}{120}$

Table 2.1: Bamboo trees coefficient

The other coefficients can not be found exactly, but we can find the linear combination between them after substituting the results from the table (2.1). In the aromatic function with three nodes $\mathcal{F}($$)$ the relation is :

$\langle b,$  $\rangle + \langle b,$  $\rangle + \langle b,$  $\rangle - \langle b,$  $\rangle = 0 \Rightarrow \langle b,$  $\rangle + \langle b,$  $\rangle = \frac{1}{3}.$

Another linear combination corresponding to the aromas with four nodes is shown in the table (2.2). By using linear algebra to find this relation, we find a system of 4 equations with 7 variables that has infinite solutions.

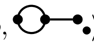
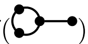
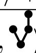
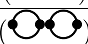
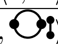
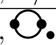
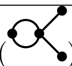
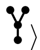
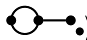
$\mathcal{F}($$)$	$\langle b,$  $\rangle + \langle b,$  $\rangle = \frac{1}{8}$
$\mathcal{F}($$)$	$\frac{1}{2}\langle b,$  $\rangle + \langle b,$  $\rangle + \langle b,$  $\rangle - \langle b,$  $\rangle = -\frac{3}{24}$
$\mathcal{F}($$)$	$\langle b,$  $\rangle - \langle b,$  $\rangle = 0$
$\mathcal{F}($$)$	$\frac{1}{2}\langle b,$  $\rangle + \langle b,$  $\rangle + \frac{1}{2}\langle b,$  $\rangle = 0$

Table 2.2: Relations between coefficients

In the same way, we can find the relation between coefficients that correspond to the aromas functions with five nodes. We find 12 equations with 26 variables. We substitute relations in the table (2.2), and rearrangement the equations, we find a system of 12 equations with 23 variables.

Conclusion

Studying volume-preserving methods has been an important topic for many years. It has been studied by Feng and Shang [11], and by Cartier and Murua [5], and by others. But it is a few articles about studying this subject by using aromatic B-series. It has been studied by Bogfjellmo [2] and by Laurent, McLachlan and Munthe-Kaas [12].

This work can help to understand how the computations take place and how the algebraic combinations between the coefficients look like. The aromatic B-series is a very useful tool in this field because it provides the divergence. In addition, using the Newton-Girard formula was useful to use with the operations on traces. To obtain the goal, it needs a huge computation on traces and vector field. By using the divergence-free vector field, we could reduce a lot of computations because the divergence sends every loop with one node to zero. Instead of using the traditional way with elementary differentials, which needs a lot of computation with a lot of concentration, using aromas methods saves a lot of effort and time.

In the Appendices, we have shown the difference between using $f^i_{j_1 \ldots j_n}$ (see A.3) and using the aromas (see A.4). To find the traces $Tr(A)$, we should do a lot of computation to obtain up to order 5. After that, we have found the conditions of the coefficients. Coefficients of the simple aromas could be found exactly. But the coefficients of the other aromas could not be found exactly. We could find the linear combinations between them. The coefficients for the aromas with five nodes were a system of 12 equations with 26 variables. We think that the combination between coefficients up to order 6 will not be linear. The method we used to find these results was by hand. For instance to find $Tr(A^2)$, we should do the multiplication $A^i_j A^j_i$. Each of these series has 12 terms with respect to the indices. This method of computation could consequence many errors. We think it will be useful in the future to find an algorithm that makes these computations easier by the computer.

Bibliography

[1] G. Bogfjellmo. Algebraic structure of aromatic B-series. *J. Comput. Dyn.*, 6(2):199–222, 2019.

[2] G. Bogfjellmo, E. Celledoni, R. McLachlan, B. Owren, and R. Quispel. Using aromas to search for preserved measures and integrals in Kahan's method. *Submitted*, 2022.

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

[4] J. C. Butcher. *B-series: algebraic analysis of numerical methods*. Springer, 2021.

[5] P. Chartier and A. Murua. Preserving first integrals and volume forms of additively split systems. *IMA J. Numer. Anal.*, 27(2):381–405, 2007.

[6] G. Fløystad, D. Manchon, and H. Z. Munthe-Kaas. The universal pre-Lie-Rinehart algebras of aromatic trees. In *Geometric and harmonic analysis on homogeneous spaces and applications*, volume 366 of *Springer Proc. Math. Stat.*, pages 137–159. Springer, Cham, [2021] ©2021.

[7] E. Hairer, C. Lubich, and G. Wanner. *Geometric numerical integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006. Structure-preserving algorithms for ordinary differential equations.

[8] R. Hirota and K. Kimura. Discretization of the Euler top. *J. Phys. Soc. Japan*, 69(3):627–630, 2000.

[9] R. Hirota and K. Kimura. Discretization of the Lagrange top. *J. Phys. Soc. Japan*, 69(10):3193–3199, 2000.

[10] A. Iserles, G. R. W. Quispel, and P. S. P. Tse. B-series methods cannot be volume-preserving. *BIT Numer. Math.*, 47(2):351–378, 2007.

[11] F. Kang and Z. J. Shang. Volume-preserving algorithms for source-free dynamical systems. *Numer. Math.*, 71(4):451–463, 1995.

[12] A. Laurent, R. I. McLachlan, H. Z. Munthe-Kaas, and O. Verdier. The aromatic bicomplex for the description of divergence-free aromatic forms and volume-preserving integrators. *Submitted*, 2023.

[13] R. I. McLachlan, K. Modin, H. Munthe-Kaas, and O. Verdier. Butcher series: a story of rooted trees and numerical methods for evolution equations. *Asia Pac. Math. Newsl.*, 7(1):1–11, 2017.

[14] H. Munthe-Kaas and O. Verdier. Aromatic Butcher series. *Found. Comput. Math.*, 16(1):183–215, 2016.

[15] B. Owren. Volume preserving methods, 2015.

[16] G. B. Thomas, M. D. Weir, J. Hass, F. R. Giordano, and R. Korkmaz. *Thomas' calculus*, volume 13. Pearson Boston, 2016.

Appendices

Appendix A

Computations of traces

The numerical solution for the system of equation (1.2) up to order 5 is after vanishing the simple aromas because of the divergence-free vector field:

$$\begin{aligned}
x_1^i = x_0^i &+ h\langle b, \bullet\rangle f^i + h^2\langle b, \rangle f^i_k f^k + h^3\langle b, \rangle(f^i_k f^k_l f^l) + \frac{h^3}{2}\langle b, \rangle(f^i_{kl} f^k f^l) + \frac{h^3}{2}\langle b, \rangle(f^k_l f^l_k f^i) \\
&+ h^4\langle b, \rangle(f^i_k f^k_l f^l_m f^m) + \frac{h^4}{6}\langle b, \rangle(f^i_{klm} f^k f^l f^m) + h^4\langle b, \rangle(f^i_{kl} f^k f^l_m f^m) \\
&+ \frac{h^4}{2}\langle b, \rangle(f^i_k f^k_{lm} f^l f^m) + \frac{h^4}{2}\langle b, \rangle(f^k_l f^l_k f^i_m f^m) + \frac{h^4}{3}\langle b, \rangle(f^k_l f^l_m f^m_k f^i) \\
&+ h^4\langle b, \rangle(f^k_{lm} f^l_k f^m f^i) + \frac{h^5}{24}\langle b, \rangle(f^i_{klmn} f^k f^l f^m f^n) + \frac{h^5}{2}\langle b, \rangle(f^i_{klm} f^k f^l f^m_n f^n) \\
&+ \frac{h^5}{2}\langle b, \rangle(f^i_{kl} f^k_m f^l_n f^m f^n) + \frac{h^5}{2}\langle b, \rangle(f^i_{nk} f^n f^k_{lm} f^l f^m) + h^5\langle b, \rangle(f^i_{nk} f^n f^k_l f^l_m f^m) \\
&+ \frac{h^5}{6}\langle b, \rangle(f^i_k f^k_{lmn} f^l f^m f^n) + h^5\langle b, \rangle(f^i_k f^k_{lm} f^l f^m_n f^n) + \frac{h^5}{2}\langle b, \rangle(f^i_k f^k_l f^l_{mn} f^m f^n) \\
&+ h^5\langle b, \rangle(f^i_k f^k_l f^l_m f^m_n f^n) + \frac{h^5}{4}\langle b, \rangle(f^l_m f^m_l f^i_{kn} f^k f^n) + \frac{h^5}{2}\langle b, \rangle(f^l_m f^m_l f^i_k f^k_n f^n) \\
&+ h^5\langle b, \rangle(f^l_{mn} f^m_l f^n f^i_k f^k) + \frac{h^5}{3}\langle b, \rangle(f^k_l f^l_m f^m_k f^i_n f^n) + \frac{h^5}{2}\langle b, \rangle(f^k_{lm} f^m f^l_{kn} f^n f^i) \\
&+ h^5\langle b, \rangle(f^k_{lm} f^l_k f^m_n f^n f^i) + h^5\langle b, \rangle(f^k_{ln} f^n f^l_m f^m_k f^i) + \frac{h^5}{4}\langle b, \rangle(f^k_l f^l_m f^m_n f^n_k f^i) \\
&+ \frac{h^5}{2}\langle b, \rangle(f^k_{lmn} f^l_k f^m f^n f^i) + \frac{h^5}{8}\langle b, \rangle(f^k_l f^l_k f^m_n f^n_m f^i) \\
&+ O(h^6).
\end{aligned} \tag{A.1}$$

Finding A^i_j:

$$\begin{aligned}
A^i_j = {} & f^i_j \\
&+ h\langle b, \rangle(f^i_{kj} f^k + f^i_k f^k_j) \\
&+ h^2\langle b, \rangle(f^i_{kj} f^k_l f^l + f^i_k f^k_{lj} f^l + f^i_k f^k_l f^l_j) \\
&+ \frac{h^2}{2}\langle b, \rangle(f^i_{klj} f^k f^l + f^i_{kl} f^k_j f^l + f^i_{kl} f^k f^l_j)
\end{aligned}$$

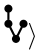
$+ \frac{h^2}{2}\langle b,$  $\rangle(f^k_{lj} f^l_k f^i + f^k_l f^l_{kj} f^i + f^k_l f^l_k f^i_j)$

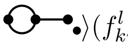
$+ h^3\langle b,$  $\rangle(f^i_{kj} f^k_l f^l_m f^m + f^i_k f^k_{lj} f^l_m f^m + f^i_k f^k_l f^l_{mj} f^m + f^i_k f^k_l f^l_m f^m_j)$

$+ \frac{h^3}{2}\langle b,$  $\rangle(f^k_{lj} f^l_k f^i_m f^m + f^k_l f^l_{kj} f^i_m f^m + f^k_l f^l_k f^i_{mj} f^m + f^k_l f^l_k f^i_m f^m_j)$

$+ \frac{h^3}{3}\langle b,$  $\rangle(f^k_{lj} f^l_m f^m_n f^i + f^k_l f^l_{mj} f^m_n f^i + f^k_l f^l_m f^m_{nj} f^i + f^k_l f^l_m f^m_n f^i_j)$

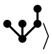
$+ \frac{h^3}{2}\langle b,$  $\rangle(f^i_{kj} f^k_{lm} f^l f^m + f^i_k f^k_{lmj} f^l f^m + f^i_k f^k_{lm} f^l_j f^m + f^i_k f^k_{lm} f^l f^m_j)$

$+ h^3\langle b,$  $\rangle(f^i_{kmj} f^k_l f^l f^m + f^i_{km} f^k_{lj} f^l f^m + f^i_{km} f^k_l f^l_j f^m + f^i_{km} f^k_l f^l f^m_j)$

$+ h^3\langle b,$  $\rangle(f^l_{kmj} f^k_l f^m f^i + f^l_{km} f^k_{lj} f^m f^i + f^l_{km} f^k_l f^m_j f^i + f^l_{km} f^k_l f^m f^i_j)$

$+ \frac{h^3}{6}\langle b,$  $\rangle(f^i_{klmj} f^k f^l f^m + f^i_{klm} f^k_j f^l f^m + f^i_{klm} f^k f^l_j f^m + f^i_{klm} f^k f^l f^m_j)$

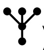
$+ \frac{h^4}{24}\langle b,$  $\rangle(f^i_{nklmj} f^n f^k f^l f^m + f^i_{nklm} f^n_j f^k f^l f^m + f^i_{nklm} f^n f^k_j f^l f^m + f^i_{nklm} f^n f^k f^l_j f^m + f^i_{nklm} f^n f^k f^l f^m_j)$

$+ \frac{h^4}{2}\langle b,$  $\rangle(f^i_{nklj} f^l_m f^m f^n f^k + f^i_{nkl} f^l_{mj} f^m f^n f^k + f^i_{nkl} f^l_m f^m_j f^n f^k + f^i_{nkl} f^l_m f^m f^n_j f^k + f^i_{nkl} f^l_m f^m f^n f^k_j)$

$+ \frac{h^4}{2}\langle b,$  $\rangle(f^i_{nkj} f^k_m f^n_l f^l f^m + f^i_{nk} f^k_{mj} f^n_l f^l f^m + f^i_{nk} f^k_m f^n_{lj} f^l f^m + f^i_{nk} f^k_m f^n_l f^l_j f^m + f^i_{nk} f^k_m f^n_l f^l f^m_j)$

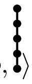
$+ \frac{h^4}{2}\langle b,$  $\rangle(f^i_{nkj} f^n f^k_{lm} f^l f^m + f^i_{nk} f^n_j f^k_{lm} f^l f^m + f^i_{nk} f^n f^k_{lmj} f^l f^m + f^i_{nk} f^n f^k_{lm} f^l_j f^m + f^i_{nk} f^n f^k_{lm} f^l f^m_j)$

$+ h^4\langle b,$  $\rangle(f^i_{nkj} f^n f^k_l f^l_m f^m + f^i_{nk} f^n_j f^k_l f^l_m f^m + f^i_{nk} f^n f^k_{lj} f^l_m f^m + f^i_{nk} f^n f^k_l f^l_{mj} f^m + f^i_{nk} f^n f^k_l f^l_m f^m_j)$

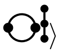
$+ \frac{h^4}{6}\langle b,$  $\rangle(f^i_{nj} f^n_{klm} f^k f^l f^m + f^i_n f^n_{klmj} f^k f^l f^m + f^i_n f^n_{klm} f^k_j f^l f^m + f^i_n f^n_{klm} f^k f^l_j f^m + f^i_n f^n_{klm} f^k f^l f^m_j)$

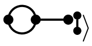
$+ h^4\langle b,$  $\rangle(f^i_{nj} f^n_{kl} f^k f^l_m f^m + f^i_n f^n_{klj} f^k f^l_m f^m + f^i_n f^n_{kl} f^k_j f^l_m f^m + f^i_n f^n_{kl} f^k f^l_{mj} f^m + f^i_n f^n_{kl} f^k f^l_m f^m_j)$

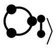
$+ \frac{h^4}{2}\langle b,$  $\rangle(f^i_{nj} f^j_k f^k_{lm} f^l f^m + f^i_n f^n_{kj} f^k_{lm} f^l f^m + f^i_n f^n_k f^k_{lmj} f^l f^m + f^i_n f^n_k f^k_{lm} f^l_j f^m + f^i_n f^n_k f^k_{lm} f^l f^m_j)$

$+ h^4\langle b,$  $\rangle(f^i_{nj} f^n_k f^k_l f^l_m f^m + f^i_n f^n_{kj} f^k_l f^l_m f^m + f^i_n f^n_k f^k_{lj} f^l_m f^m + f^i_n f^n_k f^k_l f^l_{mj} f^m + f^i_n f^n_k f^k_l f^l_m f^m_j)$

$+ \frac{h^4}{4}\langle b,$  $\rangle(f^l_{mj} f^m_l f^i_{nk} f^n f^k + f^l_m f^m_{lj} f^i_{nk} f^n f^k + f^l_m f^m_l f^i_{nkj} f^n f^k + f^l_m f^m_l f^i_{nk} f^n_j f^k + f^l_m f^m_l f^i_{nk} f^n f^k_j)$

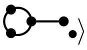
$+ \frac{h^4}{2}\langle b,$  $\rangle(f^l_{mj} f^m_l f^i_n f^n_k f^k + f^l_m f^m_{lj} f^i_n f^n_k f^k + f^l_m f^m_l f^i_{nj} f^n_k f^k + f^l_m f^m_l f^i_n f^n_{kj} f^k + f^l_m f^m_l f^i_n f^n_k f^k_j)$

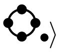
$+ h^4\langle b,$  $\rangle(f^l_{kmj} f^m f^k_l f^i_n f^n + f^l_{km} f^m_j f^k_l f^i_n f^n + f^l_{km} f^m f^k_{lj} f^i_n f^n + f^l_{km} f^m f^k_l f^i_{nj} f^n + f^l_{km} f^m f^k_l f^i_n f^n_j)$

$+ \frac{h^4}{3}\langle b,$  $\rangle(f^k_{lj} f^l_m f^m_k f^i_n f^n + f^k_l f^l_{mj} f^m_k f^i_n f^n + f^k_l f^l_m f^m_{kj} f^i_n f^n + f^k_l f^l_m f^m_k f^i_{nj} f^n + f^k_l f^l_m f^m_k f^i_n f^n_j)$

$+ \frac{h^4}{2}\langle b,$  $\rangle(f^n_{klj} f^k f^l_{nm} f^m f^i + f^n_{kl} f^k_j f^l_{nm} f^m f^i + f^n_{kl} f^k f^l_{nmj} f^m f^i + f^n_{kl} f^k f^l_{nm} f^m_j f^i + f^n_{kl} f^k f^l_{nm} f^m f^i_j)$

$+ h^4\langle b,$  $\rangle(f^k_{nlj} f^n_k f^l_m f^m f^i + f^k_{nl} f^n_{kj} f^l_m f^m f^i + f^k_{nl} f^n_k f^l_{mj} f^m f^i + f^k_{nl} f^n_k f^l_m f^m_j f^i + f^k_{nl} f^n_k f^l_m f^m f^i_j)$

$+ h^4\langle b,$  $\rangle(f^n_{kmj} f^m f^k_l f^l_n f^i + f^n_{km} f^m_j f^k_l f^l_n f^i + f^n_{km} f^m f^k_{lj} f^l_n f^i + f^n_{km} f^m f^k_l f^l_{nj} f^i + f^n_{km} f^m f^k_l f^l_n f^i_j)$

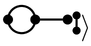
$+ \frac{h^4}{4}\langle b,$  $\rangle(f^n_{kj} f^k_l f^l_m f^m_n f^i + f^n_k f^k_{lj} f^l_m f^m_n f^i + f^n_k f^k_l f^l_{mj} f^m_n f^i + f^n_k f^k_l f^l_m f^m_{nj} f^i + f^n_k f^k_l f^l_m f^m_n f^i_j)$

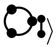
$$
\begin{aligned}
&+\frac{h^4}{2}\langle b, \rangle(f^n_{klmj}f^lf^mf^k_nf^i+f^n_{klm}f^l_jf^mf^k_nf^i+f^n_{klm}f^lf^m_jf^k_nf^i+f^n_{klm}f^lf^mf^k_{nj}f^i+f^n_{klm}f^lf^mf^k_nf^i_j)\\
&+\frac{h^4}{8}\langle b, \rangle(f^n_{kj}f^k_nf^l_mf^m_lf^i+f^n_kf^k_{nj}f^l_mf^m_lf^i+f^n_kf^k_nf^l_{mj}f^m_lf^i+f^n_kf^k_nf^l_mf^m_{lj}f^i+f^n_kf^k_nf^l_mf^m_lf^i_j)\\
&+O(h^5). \qquad \text{(A.2)}
\end{aligned}
$$

Here we will derive (2.6) with respect to (i) and after that we can find A^i_i

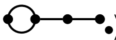
$$
\begin{aligned}
A^i_i &= h\langle b, \rangle(f^i_jf^j_i) \qquad \text{(A.3)}\\
&+h^2\langle b, \rangle(f^i_jf^j_{ki}f^k+f^i_jf^j_kf^k_i)\\
&+\frac{h^2}{2}\langle b, \rangle(f^i_{jk}f^j_if^k+f^i_{jk}f^jf^k_i+)\\
&+\frac{h^2}{2}\langle b, \rangle(f^j_{ki}f^k_jf^i+f^j_kf^k_{ji}f^i)\\
&+h^3\langle b, \rangle(f^i_jf^j_{ki}f^k_lf^l+f^i_jf^j_kf^k_{li}f^l+f^i_jf^j_kf^k_lf^l_i)\\
&+\frac{h^3}{2}\langle b, \rangle(f^k_{li}f^l_kf^i_jf^j+f^k_lf^l_{ki}f^i_jf^j f^k_lf^l_kf^i_jf^j_i)\\
&+\frac{h^3}{3}\langle b, \rangle(f^j_{ki}f^k_lf^l_jf^i+f^j_kf^k_{li}f^l_jf^i+f^j_kf^k_lf^l_{ji}f^i)\\
&+\frac{h^3}{2}\langle b, \rangle(f^i_jf^j_{kli}f^kf^l+f^i_jf^j_{kl}f^k_if^l+f^i_jf^j_{kl}f^kf^l_i)\\
&+h^3\langle b, \rangle(f^i_{jl}f^j_{ki}f^kf^l+f^i_{jl}f^j_kf^k_if^l+f^i_{jl}f^j_kf^kf^l_i)\\
&+h^3\langle b, \rangle(f^j_{kli}f^k_jf^lf^i+f^j_{kl}f^k_{ji}f^lf^i+f^j_{kl}f^k_jf^l_if^i)\\
&+\frac{h^3}{6}\langle b, \rangle(f^i_{jkl}f^j_if^kf^l+f^i_{jkl}f^jf^k_if^l+f^i_{jkl}f^jf^kf^l_i)\\
&+\frac{h^4}{24}\langle b, \rangle(f^i_{jklm}f^j_if^kf^lf^m+f^i_{jklm}f^jf^k_if^lf^m+f^i_{jklm}f^jf^kf^l_if^m+f^i_{jklm}f^jf^kf^lf^m_i)\\
&+\frac{h^4}{2}\langle b, \rangle(f^i_{jkl}f^l_{mi}f^mf^jf^k+f^i_{jkl}f^l_mf^m_if^jf^k+f^i_{jkl}f^l_mf^mf^j_if^k+f^i_{jkl}f^l_mf^mf^jf^k_i)\\
&+\frac{h^4}{2}\langle b, \rangle(f^i_{jk}f^k_{mi}f^j_lf^lf^m+f^i_{jk}f^k_mf^j_{li}f^lf^m+f^i_{jk}f^k_mf^j_lf^l_if^m+f^i_{jk}f^k_mf^j_lf^lf^m_i)\\
&+\frac{h^4}{2}\langle b, \rangle(f^i_{jk}f^j_if^k_{lm}f^lf^m+f^i_{jk}f^jf^k_{lmi}f^lf^m+f^i_{jk}f^jf^k_{lm}f^l_if^m+f^i_{jk}f^jf^k_{lm}f^lf^m_i)\\
&+h^4\langle b, \rangle(f^i_{jk}f^j_if^k_lf^l_mf^m+f^i_{jk}f^jf^k_{li}f^l_mf^m+f^i_{jk}f^jf^k_lf^l_{mi}f^m+f^i_{jk}f^jf^k_lf^l_mf^m_i)\\
&+\frac{h^4}{6}\langle b, \rangle(f^i_jf^j_{klmi}f^kf^lf^m+f^i_jf^j_{klm}f^k_if^lf^m+f^i_jf^j_{klm}f^kf^l_if^m+f^i_jf^j_{klm}f^kf^lf^m_i)\\
&+h^4\langle b, \rangle(f^i_jf^j_{kli}f^kf^l_mf^m+f^i_jf^j_{kl}f^k_if^l_mf^m+f^i_jf^j_{kl}f^kf^l_{mi}f^m+f^i_jf^j_{kl}f^kf^l_mf^m_i)\\
&+\frac{h^4}{2}\langle b, \rangle(f^i_jf^j_{ki}f^k_{lm}f^lf^m+f^i_jf^j_kf^k_{lmi}f^lf^m+f^i_jf^j_kf^k_{lm}f^l_if^m+f^i_jf^j_kf^k_{lm}f^lf^m_i)\\
&+h^4\langle b, \rangle(f^i_jf^j_{ki}f^k_lf^l_mf^m+f^i_jf^j_kf^k_{li}f^l_mf^m+f^i_jf^j_kf^k_lf^l_{mi}f^m+f^i_jf^j_kf^k_lf^l_mf^m_i)\\
&+\frac{h^4}{4}\langle b, \rangle(f^l_{mi}f^m_lf^i_{jk}f^jf^k+f^l_mf^m_{li}f^i_{jk}f^jf^k+f^l_mf^m_lf^i_{jk}f^j_if^k+f^l_mf^m_lf^i_{jk}f^jf^k_i)
\end{aligned}
$$

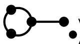
$+ \dfrac{h^4}{2}\langle b,$  $\rangle(f^l_{mi} f^m_l f^i_j f^j_k f^k + f^l_m f^m_{li} f^i_j f^j_k f^k + f^l_m f^m_l f^i_j f^j_{ki} f^k + f^l_m f^m_l f^i_j f^j_k f^k_i)$

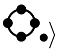
$+ h^4\langle b,$  $\rangle(f^l_{kmi} f^m f^k_l f^i_j f^j + f^l_{km} f^m_i f^k_l f^i_j f^j + f^l_{km} f^m f^k_{li} f^i_j f^j + f^l_{km} f^m f^k_l f^i_j f^j_i)$

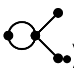
$+ \dfrac{h^4}{6}\langle b,$  $\rangle(f^k_{li} f^l_m f^m_k f^i_j f^j + f^k_l f^l_{mi} f^m_k f^i_j f^j + f^k_l f^l_m f^m_{ki} f^i_j f^j + f^k_l f^l_m f^m_k f^i_j f^j_i)$

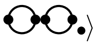
$+ \dfrac{h^4}{2}\langle b,$  $\rangle(f^j_{kli} f^k f^l_{jm} f^m f^i + f^j_{kl} f^k_i f^l_{jm} f^m f^i + f^j_{kl} f^k f^l_{jmi} f^m f^i + f^j_{kl} f^k f^l_{jm} f^m_i f^i)$

$+ h^4\langle b,$  $\rangle(f^k_{jli} f^j_k f^l_m f^m f^i + f^k_{jl} f^j_{ki} f^l_m f^m f^i + f^k_{jl} f^j_k f^l_{mi} f^m f^i + f^k_{jl} f^j_k f^l_m f^m_i f^i)$

$+ h^4\langle b,$  $\rangle(f^j_{kmi} f^m f^k_l f^l_j f^i + f^j_{km} f^m_i f^k_l f^l_j f^i + f^j_{km} f^m f^k_{li} f^l_j f^i + f^j_{km} f^m f^k_l f^l_{ji} f^i)$

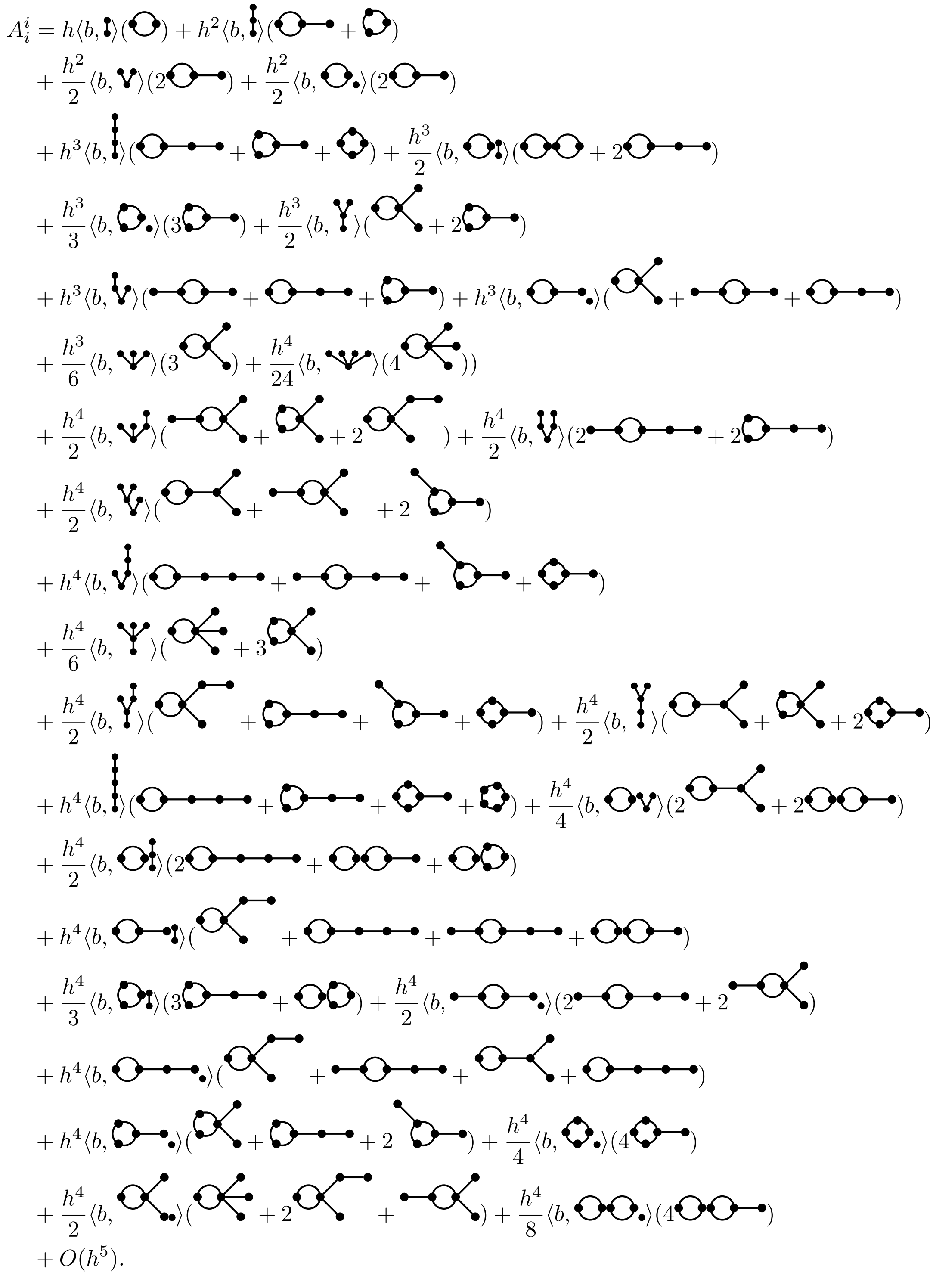
$+ \dfrac{h^4}{4}\langle b,$  $\rangle(f^j_{ki} f^k_l f^l_m f^m_j f^i + f^j_k f^k_{li} f^l_m f^m_j f^i + f^j_k f^k_l f^l_{mi} f^m_j f^i + f^j_k f^k_l f^l_m f^m_{ji} f^i)$

$+ \dfrac{h^4}{2}\langle b,$  $\rangle(f^j_{klmi} f^l f^m f^k_j f^i + f^j_{klm} f^l_i f^m f^k_j f^i + f^j_{klm} f^l f^m_i f^k_j f^i + f^j_{klm} f^l f^m f^k_{ji} f^i)$

$+ \dfrac{h^4}{8}\langle b,$  $\rangle(f^j_{ki} f^k_j f^l_m f^m_l f^i + f^j_k f^k_{ji} f^l_m f^m_l f^i + f^j_k f^k_j f^l_{mi} f^m_l f^i + f^j_k f^k_j f^l_m f^m_{li} f^i)$

$+ O(h^5).$

Now to simplify all these computations and indices writing, we will write (A.3) as aromatic functions:



(A.4)

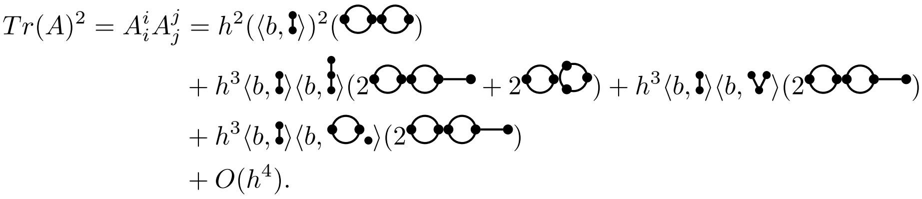
After computing of A^i_j and A^i_i, it is time to find each term of (2.7). For any fixed dimension, P can be expressed as a polynomial of traces. For example, when A is a $5\times$ 5-matrix, we have the identity (2.7)

A.1 Traces computations

Tr(A):
Find $Tr(A)$ up to order 5 as we found in (A.4):

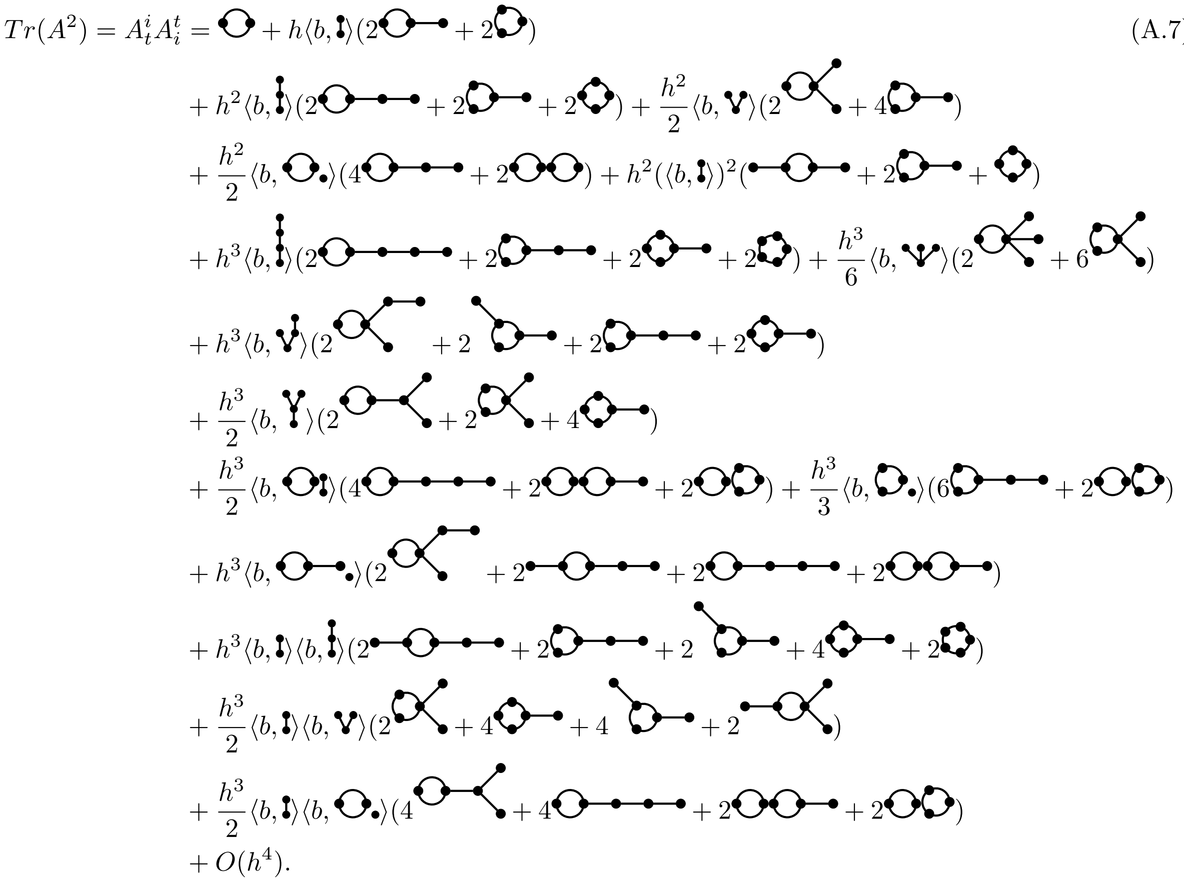
$$Tr(A) = A_i^i. \tag{A.5}$$

Find $Tr(A)^2$:



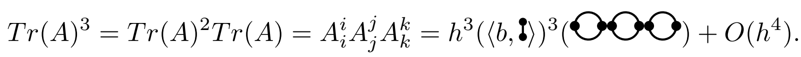
(A.6)

Finding $Tr(A^2)$



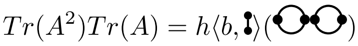
(A.7)

Finding $Tr(A)^3$



(A.8)

Finding $Tr(A^2)Tr(A)$:



(A.9)

$$+ h^2(\langle b, \rangle)^2(2 + 2) + h^2\langle b, \rangle(+) + \frac{h^2}{2}\langle b, \rangle(2) + \frac{h^2}{2}\langle b, \rangle(2) + O(h^3).$$

Finding $Tr(A^3)$

$$Tr(A^3) = A^i_j A^j_s A^s_i = + h\langle b, \rangle(3 + 3) + h^2(\langle b, \rangle)^2(3 + 6 + 3) + h^2\langle b, \rangle(3 + 3 + 3) + \frac{h^2}{2}\langle b, \rangle(3 + 6) + \frac{h^2}{2}\langle b, \rangle(6 + 3) + O(h^3). \tag{A.10}$$

Finding $Tr(A)^4$

$$Tr(A)^4 = Tr(A)^3 Tr(A) = h^4(\langle b, \rangle)^4() + O(h^5). \tag{A.11}$$

Finding $Tr(A^2)Tr(A)^2$

$$Tr(A^2)Tr(A)^2 = h^2(\langle b, \rangle)^2() + O(h^3). \tag{A.12}$$

Finding $Tr(A^2)^2$

$$Tr(A^2)^2 = Tr(A^2)Tr(A^2) = + h\langle b, \rangle(4 + 4) + O(h^2). \tag{A.13}$$

Finding $Tr(A^3)Tr(A)$

$$Tr(A^3)Tr(A) = h\langle b, \rangle() + O(h^2) \tag{A.14}$$

Finding $Tr(A^4)$

$$Tr(A^4) = A^i_j A^j_k A^k_l A^l_i = + h\langle b, \rangle(4 + 4) + O(h^2). \tag{A.15}$$

Finding $Tr(A)^5$

$$Tr(A)^5 = Tr(A)^4 Tr(A) = h^5(\langle b, \rangle)^5() + O(h^6). \tag{A.16}$$

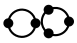
Finding $Tr(A)^3 Tr(A^2)$

$$Tr(A)^3 Tr(A^2) = h^3(\langle b, \rangle)^3() + O(h^4). \tag{A.17}$$

Finding $Tr(A^3)Tr(A)^2$

$$Tr(A^3)Tr(A)^2 = h^2(\langle b, \rangle)^2() + O(h^3). \tag{A.18}$$

Finding $Tr(A^3)Tr(A^2)$

$Tr(A^3)Tr(A^2) =$  $+ O(h)$ (A.19)

Finding $Tr(A)Tr(A^2)Tr(A^2)$

$$Tr(A)Tr(A^2)Tr(A^2) = O(h). \tag{A.20}$$

Finding $Tr(A)Tr(A^4)$

$$Tr(A)Tr(A^4) = O(h). \tag{A.21}$$

Finding $Tr(A^5)$

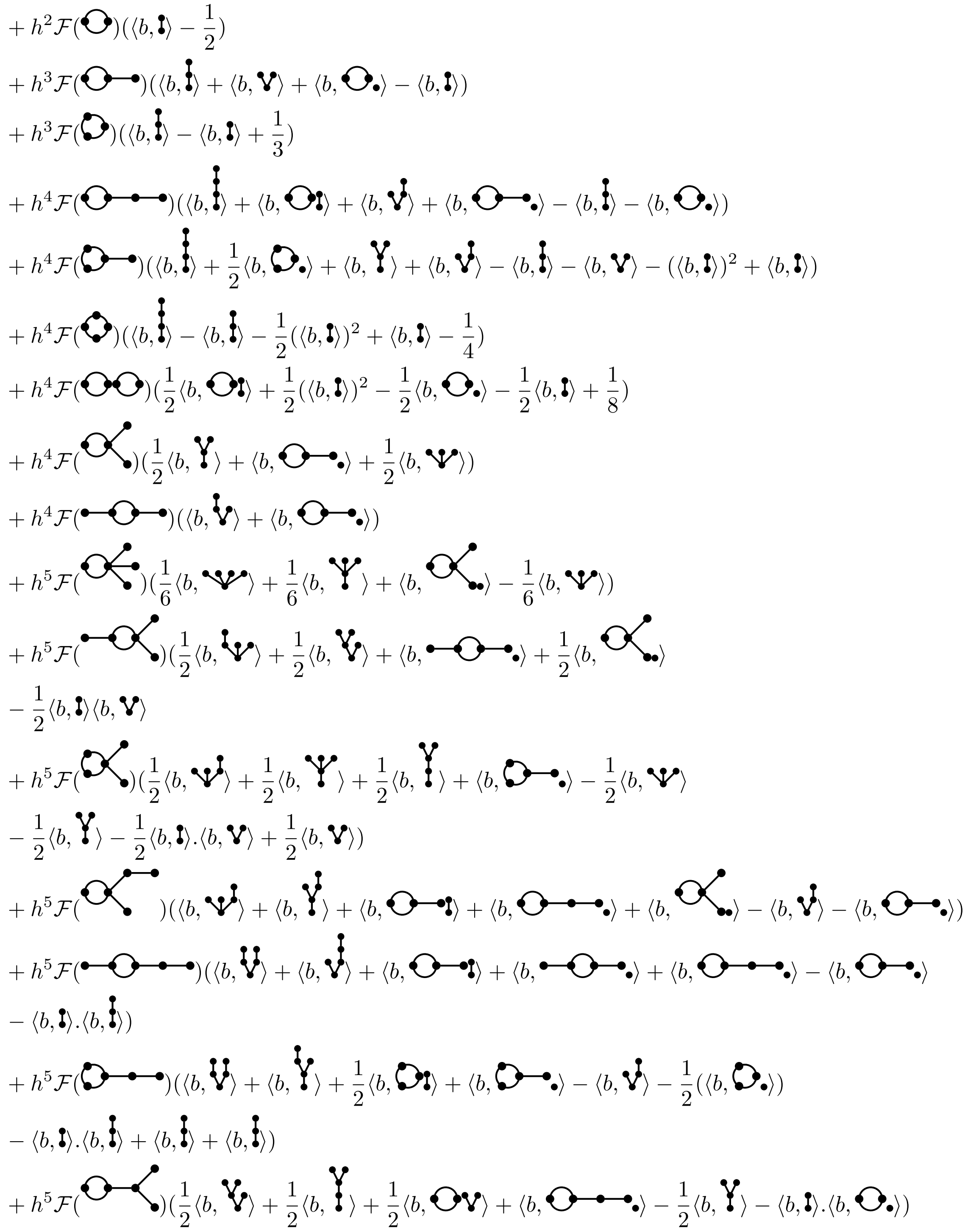
$Tr(A^5) = A^i_j A^j_k A^k_l A^l_m A^m_i =$  $+ O(h).$ (A.22)

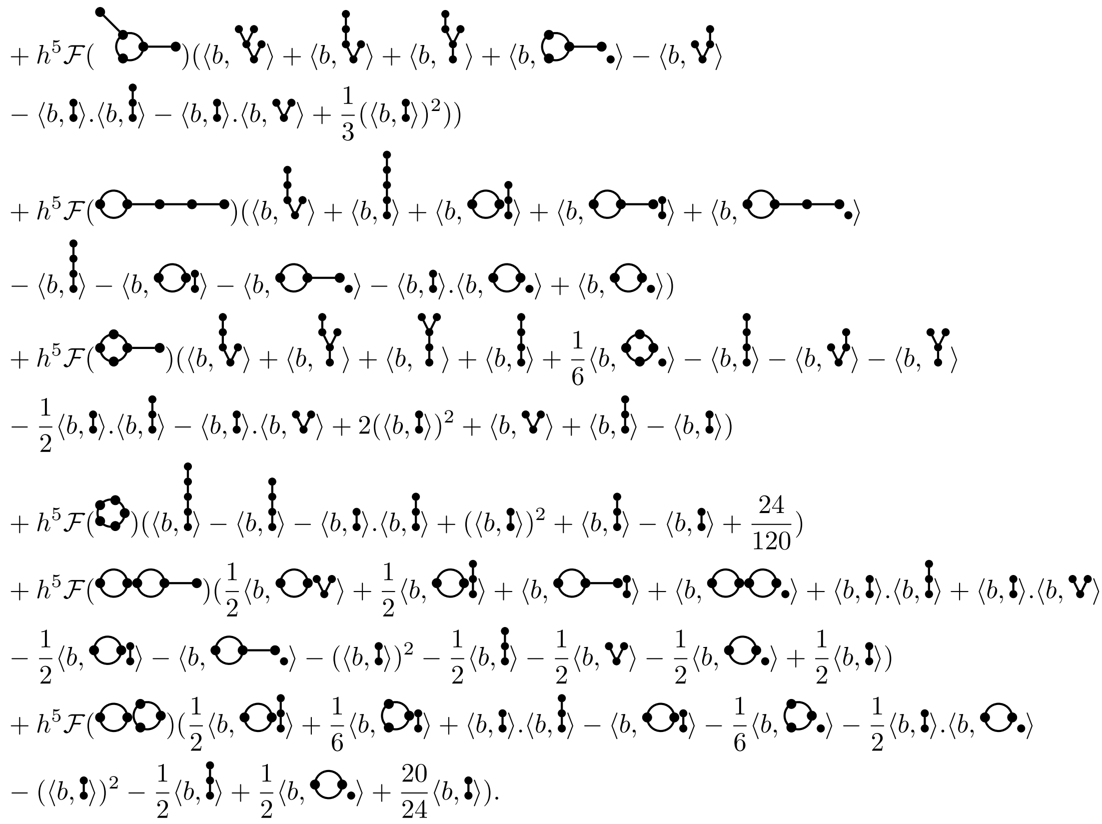
A.2 Newton-Girard formula results

det(I + hA)

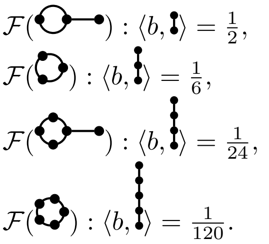
Now we substitute all traces which we have found in the formula (A.1), and collect all terms according to the aromatic function instead of coefficients, we find the following:

$$det(I + hA) = 1 \tag{A.23}$$



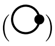
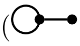


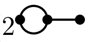
The relation between coefficients:
To obtain volume preserving, must $det(I + hA) = 1$. That means that the all term must equals to zero except the first term (1).then the coefficients of each term must equal zero. According to condition we can find the some coefficients exactly, but the another we can find a linear combination between them. The coefficients of the following functions can be found exactly

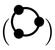
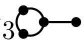
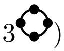


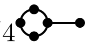
A.3 Algorithm

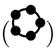
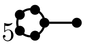
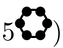
Algorithm to find $Tr(A^k)$

$k = 1 \Rightarrow \quad Tr(A) = ($$) + h\langle b,$$\rangle($$+$$) + O(h^2.$

$k = 2 \Rightarrow \quad Tr(A^2) = ($$) + h\langle b,$$\rangle(2$$+ 2$$) + O(h^2).$

$k = 3 \Rightarrow \quad Tr(A^3) = ($$) + h\langle b,$$\rangle(3$$+ 3$$) + O(h^2).$

$k = 4 \Rightarrow \quad Tr(A^4) = ($$) + h\langle b,$$\rangle(4$$+ 4$$) + O(h^2).$

$k = 5 \Rightarrow \quad Tr(A^5) = ($$) + h\langle b,$$\rangle(5$$+ 5$$) + O(h^2).$

$\vdots$

$For \quad k \Rightarrow \quad Tr(A^k) = (\lambda_k) + h\langle b,$$\rangle(k\mu_k + k\lambda_{k+1}) + O(h^2).$

where λ_k is a cycle with k nodes, μ_k is a cycle with k nodes and extra edge with one node, and k is a positive integer.

Norges miljø- og biovitenskapelige universitet
Noregs miljø- og biovitskapelege universitet
Norwegian University of Life Sciences

Postboks 5003
NO-1432 Ås
Norway