Preserving invariants and volume for split systems

Philippe Chartier\textsuperscript{1}  Ander Murua\textsuperscript{2}

\textsuperscript{1}IPSO
INRIA-Rennes and ENS Cachan, Antenne de Bretagne

\textsuperscript{2}Department of Computer Science
University of the Basque Country

Clermont 2008
Outline

1. **Problems and motivations**
   - General invariants encountered in physics
   - Improved qualitative behavior of geometric integrators

2. **Setting of the problem**
   - Invariant and volume preservation for split systems
   - The Hopf algebra of coloured trees
   - B-series and S-series for split vector fields

3. **Conditions for invariants-preservation**
   - Numerical methods preserving invariants
   - The case of quadratic and cubic invariants
   - B-series methods preserving all cubic invariants

4. **Conditions for volume-preservation**
   - Volume-preserving B-series
   - Connection with the preservation of cubic invariants
   - Volume preserving methods for split systems with a special structure

5. **From conditions for vector fields to conditions for integrators**
Outline

1. Problems and motivations
   - General invariants encountered in physics
   - Improved qualitative behavior of geometric integrators

2. Setting of the problem
   - Invariant and volume preservation for split systems
   - The Hopf algebra of coloured trees
   - B-series and S-series for split vector fields

3. Conditions for invariants-preservation
   - Numerical methods preserving invariants
   - The case of quadratic and cubic invariants
   - B-series methods preserving all cubic invariants

4. Conditions for volume-preservation
   - Volume-preserving B-series
   - Connection with the preservation of cubic invariants
   - Volume preserving methods for split systems with a special structure

5. From conditions for vector fields to conditions for integrators
Examples of first integrals

- Conservation of energy in Hamiltonian systems

Hamiltonian system

\[ \dot{p} = -\frac{\partial H}{\partial q}, \quad \dot{q} = \frac{\partial H}{\partial p}. \]

Theorem

\[ \frac{d}{dt} H(p, q) = \frac{\partial H}{\partial p} \dot{p} + \frac{\partial H}{\partial q} \dot{q} = 0 \text{ hence } H(p, q) = \text{Const} \]
Examples of first integrals

- Conservation of energy in Hamiltonian systems
- Conservation of total and angular momentum in N-Body systems

N-Body system

\[
\dot{p}_i = -\sum_{j=1}^{N} \nu_{ij} (q_i - q_j), \quad \dot{q}_i = \frac{p_i}{m_i} \quad \nu \text{ symmetric}
\]

Theorem

\[
\sum_{i=1}^{N} p_i = \text{Const and } \sum_{i=1}^{N} q_i \times p_i = \text{Const}
\]
Examples of first integrals

- Conservation of energy in Hamiltonian systems
- Conservation of total and angular momentum in N-Body systems
- Conservation of mass in chemical reactions

**Chemical reactions**

\[
\begin{align*}
A & \xrightarrow{k_1} B & \dot{y}_1 &= -k_1 y_1 + k_3 y_2 y_3 \\
B + B & \xrightarrow{k_2} B + C & \dot{y}_2 &= k_1 y_1 - k_3 y_2 y_3 - k_2 y_2^2 \\
B + C & \xrightarrow{k_3} A + C & \dot{y}_3 &= k_2 y_2^2 
\end{align*}
\]

**Theorem**

\[
\frac{d}{dt}(y_1 + y_2 + y_3) = 0 \text{ hence } l(y) = y_1 + y_2 + y_2 = \text{Const.}
\]
General invariants encountered in physics

Examples of first integrals

- Conservation of energy in Hamiltonian systems
- Conservation of total and angular momentum in N-Body systems
- Conservation of mass in chemical reactions
- Conservation of the spectrum by matrix flows

Isospectral matrix equations

\[ \dot{L} = B(L) L - L B(L) \text{ with } B(L) \text{ skew-symmetric.} \]

Theorem

Let \( \dot{U} = B(L(t))U, \ U(0) = I. \) Then, \( L(t) = U(t)L_0 U(t)^{-1}. \)
Examples of first integrals

- Conservation of energy in Hamiltonian systems
- Conservation of total and angular momentum in N-Body systems
- Conservation of mass in chemical reactions
- Conservation of the spectrum by matrix flows
- Conservation of volume in divergence-free systems

Divergence-free system

\[ \dot{y} = f(y) \text{ with } \text{div}(f) = 0.\]

Theorem

The flow \( \varphi_t \) preserves the volume, i.e.

\[ \int_{\varphi_t(A)} dy = \int_A dy. \]
Improved qualitative behavior of geometric integrators

A prey-predator model in normal form

\[
\begin{align*}
\dot{U} &= e^V - 2 = f(V) \\
\dot{V} &= 1 - e^U = g(U)
\end{align*}
\]
A prey-predator model in normal form

\[
\begin{align*}
\dot{U} &= e^V - 2 = f(V) \\
\dot{V} &= 1 - e^U = g(U)
\end{align*}
\]
Improved qualitative behavior of geometric integrators

2-D Kepler Problem

\[ H(p, q) = \frac{1}{2} p^T p - \frac{1}{\sqrt{q^T q}} = T(p) + V(q) \quad \iff \quad \ddot{q} = -V'(q). \]
Improved qualitative behavior of geometric integrators

2-D Kepler Problem

\[ H(p, q) = \frac{1}{2} p^T p - \frac{1}{\sqrt{q^T q}} = T(p) + V(q) \Longleftrightarrow \ddot{q} = -V'(q). \]
Improved qualitative behavior of geometric integrators

2-D Kepler Problem

\[ H(p, q) = \frac{1}{2} p^T p - \frac{1}{\sqrt{q^T q}} = T(p) + V(q) \iff \ddot{q} = -V'(q). \]
Outline

1. Problems and motivations
   - General invariants encountered in physics
   - Improved qualitative behavior of geometric integrators

2. Setting of the problem
   - Invariant and volume preservation for split systems
   - The Hopf algebra of coloured trees
   - B-series and S-series for split vector fields

3. Conditions for invariants-preservation
   - Numerical methods preserving invariants
   - The case of quadratic and cubic invariants
   - B-series methods preserving all cubic invariants

4. Conditions for volume-preservation
   - Volume-preserving B-series
   - Connection with the preservation of cubic invariants
   - Volume preserving methods for split systems with a special structure

5. From conditions for vector fields to conditions for integrators
The two classes of problems considered

We consider systems of ODEs of the form

\[ \dot{y} = f[1](y) + f[2](y) + \ldots + f[N](y), \]

such that each individual vector field has the invariant function \( I \)

\[ 0 = (\nabla_y I(y))^T f[\nu](y), \quad \nu = 1, \ldots, N, \]
The two classes of problems considered

We consider systems of ODEs of the form

\[ \dot{y} = f^{[1]}(y) + f^{[2]}(y) + \ldots + f^{[N]}(y), \]

Split vector fields systems

or preserves the volume form

Divergence-free

\[ 0 = \text{div } f^{[\nu]}(y), \quad \nu = 1, \ldots, N \]
Invariant and volume preservation for split systems

Invariant preserving integrators

A one-step method

is a map from the phase-space to itself, which, given an approximation $y$ of the solution at time $t$, produces an approximation $\Phi^f_h$ at time $t + h$.

The modified vector field

associated to a numerical integrator $\Phi^f_h$ is the vector field $\tilde{f}_h$ such that the exact solution of $\dot{z} = \tilde{f}_h(z)$, $z(t) = y$ at time $t + h$ is $\Phi^f_h(y)$.

Invariant-preserving integrators (1)

$\Phi^f_h$ preserves $I$ if $I(\Phi^f_h(y)) = I(y)$ for any $y$. 
Invariant and volume preservation for split systems

Invariant preserving integrators

A one-step method

is a map from the phase-space to itself, which, given an approximation $y$ of the solution at time $t$, produces an approximation $\Phi^f_h$ at time $t + h$.

The modified vector field

associated to a numerical integrator $\Phi^f_h$ is the vector field $\tilde{f}_h$ such that the exact solution of $\dot{z} = \tilde{f}_h(z), \ z(t) = y$ at time $t + h$ is $\Phi^f_h(y)$.

Invariant-preserving integrators (2)

$\Phi^f_h$ preserves $l$ if $(\nabla l(y))^T \tilde{f}_h(y) = 0$ for any $y$. 
Volume-preserving integrators

**A one-step method**

is a map from the phase-space to itself, which, given an approximation $y$ of the solution at time $t$, produces an approximation $\Phi^f_h(y)$ at time $t + h$.

**The modified vector field**

associated to a numerical integrator $\Phi^f_h$ is the vector field $\tilde{f}_h$ such that the exact solution of $\dot{z} = \tilde{f}_h(z), \quad z(t) = y$ at time $t + h$ is $\Phi^f_h(y)$.

**Volume-preserving integrators**

$\Phi^f_h$ preserves the volume if $\det \left( \frac{\partial \Phi^f_h(y)}{\partial y} \right) = 1$ for any $y$. 
Volume-preserving integrators

A one-step method

is a map from the phase-space to itself, which, given an approximation $y$ of the solution at time $t$, produces an approximation $\Phi^f_h(y)$ at time $t + h$.

The modified vector field

associated to a numerical integrator $\Phi^f_h$ is the vector field $\tilde{f}_h$ such that the exact solution of $\dot{z} = \tilde{f}_h(z)$, $z(t) = y$ at time $t + h$ is $\Phi^f_h(y)$.

Volume-preserving integrators (2)

$\Phi^f_h$ preserves the volume if $\text{div} \left( \tilde{f}_h(y) \right) = 0$ for any $y$. 
Volume-preserving integrators

**A one-step method**

is a map from the phase-space to itself, which, given an approximation $y$ of the solution at time $t$, produces an approximation $\Phi^f_h(y)$ at time $t + h$.

**The modified vector field**

associated to a numerical integrator $\Phi^f_h$ is the vector field $\tilde{f}_h$ such that the exact solution of $\dot{z} = \tilde{f}_h(z)$, $z(t) = y$ at time $t + h$ is $\Phi^f_h(y)$.

The conditions for preserving the volume are easier to obtain in terms of the modified vector field.
The Hopf algebra of coloured trees

Trees and forests [Merson 57, Butcher 68]

**Definition**

The set of trees $\mathcal{T}$ and forests $\mathcal{F}$ are defined recursively by:

1. $e \in \mathcal{F}$
2. If $t_1, \ldots, t_n \in \mathcal{T}^n$, then $u = t_1 \ldots t_n \in \mathcal{F}$
3. If $u \in \mathcal{F}$ and $\nu \in \{1, \ldots, N\}$, then $t = [u]_\nu = B^{+}_\nu(u) \in \mathcal{T}$.

**Example**

\[ B^{+}_1(\bullet \circ) = \begin{bmatrix} \circ \circ \end{bmatrix}_1 = \circ \circ \text{ and } B^{+}_2(\bullet \bullet) = \begin{bmatrix} \bullet \bullet \end{bmatrix}_2 = \bullet \bullet \]

\[ B^{-}(\circ \circ) = \bullet \bullet \text{ and } B^{-}(\bullet \circ \bullet) = \circ \circ \]

\[ B^{-}(\circ \bullet) = \bullet \circ \text{ and } B^{-}(\bullet \circ \circ) = \circ \bullet \]
The Hopf algebra of coloured trees

Order and symmetry

**Definition**

Consider $n$ distinct trees $t_1, \ldots, t_n$ and let $u = t_1^{r_1} \ldots t_n^{r_n}$ and $t = [u]_\nu$. Then,

- $|t| = 1 + |u| = 1 + r_1|t_1| + \ldots + r_n|t_n|$
- $\sigma(u) = r_1! \ldots r_n! (\sigma(t_1))^{r_1} \ldots (\sigma(t_n))^{r_n}$ and $\sigma(t) = \sigma(u)$

**Example**

<table>
<thead>
<tr>
<th>Forest $u$</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Order $</td>
<td>u</td>
<td>$</td>
<td>4</td>
</tr>
<tr>
<td>Symmetry $\sigma(u)$</td>
<td>2!</td>
<td>1! 3! 1!</td>
<td>3!(2!)³ 2!</td>
</tr>
</tbody>
</table>
The Hopf algebra of coloured trees

Structure (Connes and Kreimer 98, Brouder 04)

**Definition**

The set $\mathcal{F}$ can be naturally endowed with an algebra structure $\mathcal{H}$ on $\mathbb{R}$:

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

**Calculus in $\mathcal{H}$**

\[
(2 \cdot \begin{array}{c} \bullet \\ + 3 \end{array} + 8 \cdot ) (\begin{array}{c} \bullet \\ - \end{array} - \begin{array}{c} \bullet \\ + \end{array} + 8 \cdot ) = 2 \cdot \begin{array}{c} \bullet \\ \end{array} \begin{array}{c} \bullet \\ \end{array} - 2 \cdot \begin{array}{c} \bullet \\ \end{array} \begin{array}{c} \bullet \\ \end{array} + 16 \cdot \begin{array}{c} \bullet \\ \end{array}.
\]

\[
+ 3 \cdot \begin{array}{c} \bullet \\ \end{array} \begin{array}{c} \bullet \\ \end{array} - 3 \cdot \begin{array}{c} \bullet \\ \end{array} \begin{array}{c} \bullet \\ \end{array} + 24 \cdot \begin{array}{c} \bullet \\ \end{array}.
\]
The co-product

Definition

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

\[
\begin{align*}
(\lambda u + \mu v) \otimes w &= \lambda (u \otimes w) + \mu (v \otimes w), \\
w \otimes (\lambda u + \mu v) &= \lambda (w \otimes u) + \mu (w \otimes v), \\
(u \otimes v)(w \otimes x) &= (uw \otimes vx).
\end{align*}
\]

Definition

The co-product $\Delta$ is a morphism from $\mathcal{H}$ to $\mathcal{H} \otimes \mathcal{H}$ defined by:

1. $\Delta(e) = e \otimes e$,
2. $\forall t \in \mathcal{T}, \Delta(t) = t \otimes e + (id_{\mathcal{H}} \otimes B^+_{\mu(t)}) \circ \Delta \circ B^-(t)$,
3. $\forall u = t_1 \ldots t_n \in \mathcal{F}, \Delta(u) = \Delta(t_1) \ldots \Delta(t_n)$. 
The Hopf algebra of coloured trees

The co-product

Example

\[ \Delta(\mathcal{V}) = \mathcal{V} \otimes e + (id \otimes B_2^+) \Delta(\cdot \circ) \]
\[ = \mathcal{V} \otimes e + (id \otimes B_2^+) \Delta(\cdot) \Delta(\circ) \]
\[ = \mathcal{V} \otimes e + (id \otimes B_2^+) (\cdot \otimes e + e \otimes \cdot) (\circ \otimes e + e \otimes \circ) \]
\[ = \mathcal{V} \otimes e + (id \otimes B_2^+) (\cdot \circ e + \cdot \circ \circ + \circ \circ \circ + e \circ \circ \circ) \]
\[ = \mathcal{V} \otimes e + \cdot \circ \circ \circ + \cdot \circ \mathcal{V} + \circ \circ \mathcal{V} + e \circ \mathcal{V} \]
**Elementary differentials**

**Definition**

Let $t$ be a tree of $\mathcal{T}$. The elementary differential $F(t)$ associated with $t$ is the mapping from $\mathbb{R}^n$ to $\mathbb{R}^n$, defined by:

1. $F(\nu)(y) = f^{[\nu]}(y)$,
2. $F([t_1, \ldots, t_n]_\nu)(y) = (f^{[\nu]})^{(n)}(y) \left(F(t_1)(y), \ldots, F(t_n)(y)\right)$.

**Example**

- $F(\nu) = (f^{[1]})' f^{[2]}$
- $F(\nu_1) = (f^{[2]})''(y) (f^{[1]}, f^{[2]})$
- $F(\nu_2) = (f^{[1]})' (f^{[2]})' f^{[1]}$
Elementary differential operators

**Definition**

Let $u = t_1 \ldots t_k$ be a forest of $\mathcal{F}$. The differential operator $X(u)$ associated with $u$ is defined on $\mathcal{D} = C^\infty(\mathbb{R}^n; \mathbb{R}^m)$ by:

$$X(u) : \mathcal{D} \to \mathcal{D}$$

$$g \mapsto X(u)[g] = g^{(k)}(F(t_1), \ldots, F(t_k)).$$

**Example**

$$X(e)[g] = g$$
$$X(\cdot)[g] = g' f^{[1]}$$
$$X(\circ)[g] = g' (f^{[1]})' f^{[2]}$$
$$X(\bullet \circ \bullet)[g] = g^{(3)}((f^{[1]})' f^{[1]}, f^{[2]}, f^{[1]})$$
B-series and S-series for split vector fields

**B-series and S-series**

**Definition (B-Series (Hairer and Wanner 74))**

Let $a : \mathcal{T} \rightarrow \mathbb{R}$. The B-series $B(a, y)$ is the formal series:

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

**Example (Implicit/Explicit Euler)**

$$y_1 = y_0 + h \left( f^{[1]}(y_1) + f^{[2]}(y_0) \right)$$

$$= y_0 + hF(\cdot)(y_0) + hF(\circ)(y_0) + h^2 F(\bullet)(y_0) + h^2 F(\circlearrowright)(y_0) + \ldots$$
B-series and S-series for split vector fields

B-series and S-series

**Definition (Series of differential operators)**

Let \( \alpha : \mathcal{F} \to \mathbb{R} \). The S-series \( S(\alpha) \) is the formal series

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

**Example (Implicit/Explicit Euler)**

\[
g(y_1) = g \left( y_0 + hf^{[1]}(y_1) + hf^{[2]}(y_0) \right)
\]

\[
= X(e)[g] + h(X(\cdot)[g] + X(\circ)[g]) + h^2(X(\cdot)[g] + X(\circ)[g])
\]

\[
+ \frac{h^2}{2} \left( X(\cdot^2)[g] + 2X(\cdot \circ)[g] + X(\circ^2)[g] \right) + \ldots
\]
Composition of series and co-product in $\mathcal{H}$

**Theorem (Composition of B-series)**

Let $a$ and $b$ be two mappings from $\mathcal{T}$ to $\mathbb{R}$. The composition of the two B-series $B(a, y)$ and $B(b, y)$, i.e. $B(b, B(a, y))$, is again a B-series $B(a \cdot b, y)$, with coefficients $a \cdot b$ defined on $\mathcal{T}$ by

$$\forall t \in \mathcal{T}, \quad (a \cdot b)(t) = (\mu_{\mathbb{R}} \circ (a \otimes b) \circ \Delta)(t).$$

**Example**

$$(a \cdot b)(\mathcal{V}) = \mu_{\mathbb{R}} \circ (a \otimes b) \left( \mathcal{V} \otimes e + \bullet \otimes o + \bullet \otimes \mathcal{I} + o \otimes \mathcal{I} + e \otimes \mathcal{V} \right)$$

$$= a(\mathcal{V})b(e) + a(\bullet)a(o)b(\bullet) + a(\bullet)b(\mathcal{I}) + a(o)b(\mathcal{I}) + a(e)b(\mathcal{V})$$
Composition of series and co-product in $\mathcal{H}$

**Theorem (Composition of S-series)**

Let $\alpha$ and $\beta$ be two mappings from $\mathcal{F}$ to $\mathbb{R}$. The composition of the two S-series $S(\alpha)$ and $S(\beta)$, i.e. $S(\alpha)[S(\beta)[.]$] is again a S-series, with coefficients $\alpha \cdot \beta$ defined on $\mathcal{F}$ by

$$\forall u \in \mathcal{F}, \quad (\alpha \beta)(u) = (\mu_\mathbb{R} \circ (\alpha \otimes \beta) \circ \Delta)(u).$$

**Example**

$$(\alpha \cdot \beta)(\begin{array}{c} \mathcal{H} \\ \end{array}) = \mu_\mathbb{R} \circ (\alpha \otimes \beta) \bigg( \begin{array}{c} \mathcal{H} \\ \end{array} \otimes e + \begin{array}{c} \mathcal{H} \\ \end{array} \otimes \begin{array}{c} \mathcal{H} \\ \end{array} + \begin{array}{c} \mathcal{H} \\ \end{array} \otimes \begin{array}{c} \mathcal{H} \\ \end{array} + e \otimes \begin{array}{c} \mathcal{H} \\ \end{array} \bigg)$$

$$= \alpha(\begin{array}{c} \mathcal{H} \\ \end{array})\beta(e) + \alpha(\begin{array}{c} \mathcal{H} \\ \end{array})\beta(\begin{array}{c} \mathcal{H} \\ \end{array}) + \alpha(\begin{array}{c} \mathcal{H} \\ \end{array})\beta(\begin{array}{c} \mathcal{H} \\ \end{array}) + \alpha(\begin{array}{c} \mathcal{H} \\ \end{array})\beta(\begin{array}{c} \mathcal{H} \\ \end{array}) + \alpha(e)\beta(\begin{array}{c} \mathcal{H} \\ \end{array})$$
Outline

1. Problems and motivations
   - General invariants encountered in physics
   - Improved qualitative behavior of geometric integrators

2. Setting of the problem
   - Invariant and volume preservation for split systems
   - The Hopf algebra of coloured trees
   - B-series and S-series for split vector fields

3. Conditions for invariants-preservation
   - Numerical methods preserving invariants
   - The case of quadratic and cubic invariants
   - B-series methods preserving all cubic invariants

4. Conditions for volume-preservation
   - Volume-preserving B-series
   - Connection with the preservation of cubic invariants
   - Volume preserving methods for split systems with a special structure

5. From conditions for vector fields to conditions for integrators
   - Substitution law
The action of a function $I$ on a B-series

It can be viewed as S-series:

$$I(B(a, y)) = S(\alpha)[l] \iff \alpha \in Alg(\mathcal{H}, \mathbb{R}) \text{ and } \alpha|_T \equiv a.$$ 

A B-series integrator $B(a, y)$ preserves $I$ iff

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

i.e.

$$S(\alpha)[l] = l,$$

where $\alpha$ is the unique algebra-morphism extending $a$ onto $\mathcal{H}$. 

Numerical methods preserving invariants

The annihilating left ideal $I/l$ of $l$

Using the assumption of a common invariant $l$

For $\nu = 1, \ldots, N$, $X(\cdot_\nu)[l] = (\nabla l)f[\nu] = 0$. Hence,

$$\sum_{\nu=1}^{N} S(\omega_\nu)[hX(\cdot_\nu)[l]] = S(\omega')[l] = 0.$$ 

Lemma

For any $(\omega_1, \ldots, \omega_N) \in (\mathcal{H}^*)^N$, we have $\omega'(e) = 0$ and

$$\forall u = t_1 \cdots t_m \in \mathcal{F}, \quad \omega'(u) = \sum_{i=1}^{m} \omega_{\mu(t_i)} \left( B^{-}(t_i) \prod_{j \neq i} t_j \right).$$
Problems and motivations
Setting of the problem
Conditions for invariants-preservation
Conditions for volume-preservation

Numerical methods preserving invariants

Integrators preserving general invariants

Theorem

Let $\alpha \in \text{Alg}(\mathcal{H}, \mathbb{R})$. Then $\alpha$ satisfies $S(\alpha)[I] = 1$ that for all couples $(f, I)$ of a vector field $f$ and a first integral $I$, if and only if $\alpha(e) = 1$ and $\alpha$ satisfies the condition

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

for all $m \geq 2$ and all $t_i$’s in $\mathcal{T}$.

Theorem

Let $\beta \in \text{VF}(\mathcal{H}, \mathbb{R})$. Then $\beta$ satisfies $S(\beta)[I] = 0$ that for all couples $(f, I)$ if and only if $\alpha$ satisfies the condition

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

for all $m \geq 2$ and all $t_i$’s in $\mathcal{T}$.
For quadratic first integral $I$, the condition becomes

$$\forall (t_1, t_2) \in T^2, \quad b(t_1 \circ t_2) + b(t_2 \circ t_1) = 0.$$ 

while for cubic invariants $I$, one needs in addition that

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

Theorem

A B-series integrator that preserves all cubic polynomial invariants does in fact preserve polynomial invariants of any degree and can be formally interpreted as the exact flow of a vector field lying in the Lie-algebra generated by $f^{[1]}, \ldots, f^{[N]}$. 
Outline

1. Problems and motivations
   - General invariants encountered in physics
   - Improved qualitative behavior of geometric integrators

2. Setting of the problem
   - Invariant and volume preservation for split systems
   - The Hopf algebra of coloured trees
   - B-series and S-series for split vector fields

3. Conditions for invariants-preservation
   - Numerical methods preserving invariants
   - The case of quadratic and cubic invariants
   - B-series methods preserving all cubic invariants

4. Conditions for volume-preservation
   - Volume-preserving B-series
   - Connection with the preservation of cubic invariants
   - Volume preserving methods for split systems with a special structure

5. From conditions for vector fields to conditions for integrators
Split systems with zero-divergence

Divergence-free B-series

For systems of the form

\[ \dot{y} = \sum_{\nu=1}^{N} f^{[\nu]}(y) \text{ with } \text{div} f^{[\nu]} = 0, \]

a B-series modified vector field is divergence free if

\[ \text{div}(h\tilde{f}_h(y)) = \sum_{t \in T} \frac{h^{|t|}}{\sigma(t)} b(t) \text{div}(F(t)(y)) = 0. \]

Question

How to compute and represent the terms in \( \text{div}(F(t)(y)) \)?
Volume-preserving B-series

A convenient formula for the derivative of an elementary differential

### Notation

For $t = [t_1, \ldots, t_l] \nu \in \mathcal{T}$, $F^*(t) = \frac{\partial^{l+1} f[\nu]}{\partial y^{l+1}} (F(t_1), \ldots, F(t_l))$.

### The formula

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

The grafting operation is meant to operate from right to left.

$$\frac{\text{div}(F(t))}{\sigma(t)} = \frac{\text{Tr}(F^*(t))}{\sigma(t)} + \sum_{t_1 \circ t_2 \circ \cdots \circ t_m = t} \frac{\text{Tr}(F^*(t_1) \cdots F^*(t_m))}{\sigma(t_1) \cdots \sigma(t_m)}.$$
The set of aromatic trees $\mathcal{AT}$

**Definition**

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

\[ o = \quad = (t_1 t_2 t_1 t_2) \quad \quad t_1 = \quad = \quad t_2 = \quad = \]
1-cuts of aromatic trees

**Definition**

For any aromatic tree $\mathbf{o} = (t_1 \ldots t_m) \in \mathcal{AT}$, $C(\mathbf{o})$ is the unordered list of trees obtained from $\mathbf{o}$ by breaking any edge of the cycle. If we denote for $i = 1, \ldots, m$, 

$$s_i = t_i \circ t_{i+1} \circ \ldots \circ t_m \circ t_1 \circ \ldots \circ t_{i-1},$$

then:

$$C(\mathbf{o}) = \{s_1, \ldots, s_m\}. \quad (1)$$

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

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

so that, for each $i$, there are $\theta$ copies of $s_i$ in the list $C(\mathbf{o})$. Then the symmetry coefficient of $\mathbf{o}$ is defined as $\sigma(\mathbf{o}) = \theta \prod_i \sigma(t_i)$. 
The list \( C(o) = \{ s_1, s_2, s_3, s_4 \} \) for \( o = (t_1t_2t_1t_2) \)

\[
\begin{align*}
\mathcal{S}_1 &= t_1 \circ t_2 \circ t_1 \circ t_2, \\
\mathcal{S}_2 &= t_2 \circ t_1 \circ t_2 \circ t_1, \\
\mathcal{S}_3 &= t_1 \circ t_2 \circ t_1 \circ t_2, \\
\mathcal{S}_4 &= t_2 \circ t_1 \circ t_2 \circ t_1 =
\end{align*}
\]
Divergence of a B-series vector field

Definition (Elementary divergence)

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

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

Collecting the terms

$$\text{div}(B(b)) = \sum_{t \in T} b(t) h^{|t|} \sum_{m \geq 2} \sum_{t_1 \cdots t_m = t} \frac{\text{div}((t_1 \ldots t_m))}{\sigma(t_1) \cdots \sigma(t_m)}$$

$$= \sum_{n \geq 2} h^n \sum_{o \in AT_n} \left( \sum_{t \in C(o)} b(t) \right) \frac{\text{div}(o)}{\sigma(o)}.$$
Divergence-free conditions

**Theorem**

*A modified field given by the B-series $B(b, y)$ is divergence-free up to order $p$ if the following condition is satisfied:*

$$
\sum_{t \in C(o)} b(t) = 0 \text{ for all } o \in AT \text{ with } |o| \leq p.
$$

**Example**

For $o = (t_1 t_2 t_1 t_2)$,

$$
2b(t_1 \circ t_2 \circ t_1 \circ t_2) + 2b(t_2 \circ t_1 \circ t_2 \circ t_1) = 0.
$$
2-3 cycles conditions and conditions for quadratic/cubic invariants

1. 2-cycles clearly coincide with the conditions for quadratic invariants.

2. for 3-cycles conditions

\[
0 = b(t_1 \circ t_2 \circ t_3) + b(t_2 \circ t_1 \circ t_3) + b(t_3 \circ t_2 \circ t_1),
\]
\[
= b(t_1 \circ (t_2 \circ t_3)) + b(t_2 \circ (t_1 \circ t_3)) + b(t_3 \circ (t_2 \circ t_1)),
\]
\[
= -b((t_2 \circ t_3) \circ t_1) - b((t_1 \circ t_3) \circ t_2) - b((t_2 \circ t_1) \circ t_3),
\]
\[
= -b(t_2 \circ t_1 t_3) - b(t_1 \circ t_2 t_3) - b(t_2 \circ t_1 t_3).
\]

Theorem

A volume-preserving B-series integrator can be formally interpreted as the exact flow of a vector field lying in the Lie-algebra generated by \( f^{[1]}, \ldots, f^{[N]} \).
volume preserving methods for split systems with a special structure

The conditions for a special class of systems

3-cycle systems

\[
\begin{pmatrix}
\dot{p} \\
\dot{q} \\
\dot{r}
\end{pmatrix}
= 
\begin{pmatrix}
\mathcal{F}(q) \\
\mathcal{G}(r) \\
\mathcal{H}(p)
\end{pmatrix}
= f[1](q) + f[2](r) + f[3](p).
\]

Black trees

For \( u = [v_1, \ldots, v_m] \), one has

\[
F^*(u) = \frac{\partial^{m+1} f[1]}{\partial (p, q, r)^{m+1}}(F(v_1), \ldots, F(v_m)) = 
\begin{pmatrix}
0 & \times & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.
\]
The conditions for a special class of systems

### 3-cycle systems

\[
\begin{pmatrix}
\dot{p} \\
\dot{q} \\
\dot{r}
\end{pmatrix} = \begin{pmatrix}
F(q) \\
G(r) \\
H(p)
\end{pmatrix} = f^{[1]}(q) + f^{[2]}(r) + f^{[3]}(p).
\]

### White trees

For \( v = [w_1, \ldots, w_n] \), one has

\[
F^*(v) = \frac{\partial^{n+1} f^{[2]}}{\partial (p, q, r)^{n+1}}(F(w_1), \ldots, F(w_n)) = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & \times \\
0 & 0 & 0
\end{pmatrix}.
\]
The conditions for a special class of systems

3-cycle systems

\[
\begin{pmatrix}
\dot{p} \\
\dot{q} \\
\dot{r}
\end{pmatrix}
= \begin{pmatrix}
\mathcal{F}(q) \\
\mathcal{G}(r) \\
\mathcal{H}(p)
\end{pmatrix}
= f^{[1]}(q) + f^{[2]}(r) + f^{[3]}(p).
\]

Square trees

For \( w = [u_1, \ldots, u_r] \square \), one has

\[
F^*(w) = \frac{\partial^{r+1} f^{[3]}}{\partial (p, q, r)^{r+1}}(F(w_1), \ldots, F(w_n)) = \begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
\times & 0 & 0
\end{pmatrix}.
\]
The conditions for a special class of systems

3-cycle systems

\[
\begin{pmatrix}
\dot{p} \\
\dot{q} \\
\dot{r}
\end{pmatrix} = \begin{pmatrix}
F(q) \\
G(r) \\
H(p)
\end{pmatrix} = f[1](q) + f[2](r) + f[3](p).
\]

Consequence

\[
\text{div}(o) \neq 0 \text{ iff } o = (u_1 v_1 w_1 u_2 v_2 w_2 \ldots u_m v_m w_m), \ m \geq 1.
\]
Volume-preserving RK-methods for 3-cycle systems

Theorem

A one-stage additive Runge-Kutta method formed of 
\((A^{[i]}, b^{[i]}) = (\theta_i, 1), i = 1, 2, 3,\) is volume-preserving for 3-cycle systems iff

\[(\theta_1 - 1)(\theta_2 - 1)(\theta_3 - 1) = \theta_1\theta_2\theta_3.\]

Example

An implicit "non-symplectic" RK-method

\[
\begin{align*}
P &= p_0 + \frac{h}{3} F(Q) & p_1 &= p_0 + hF(Q) \\
Q &= q_0 + \frac{4h}{3} G(R) & q_1 &= q_0 + hG(R) \\
R &= r_0 + \frac{h}{3} H(P) & p_1 &= p_0 + hH(P)
\end{align*}
\]
Outline

1. Problems and motivations
   - General invariants encountered in physics
   - Improved qualitative behavior of geometric integrators

2. Setting of the problem
   - Invariant and volume preservation for split systems
   - The Hopf algebra of coloured trees
   - B-series and S-series for split vector fields

3. Conditions for invariants-preservation
   - Numerical methods preserving invariants
   - The case of quadratic and cubic invariants
   - B-series methods preserving all cubic invariants

4. Conditions for volume-preservation
   - Volume-preserving B-series
   - Connection with the preservation of cubic invariants
   - Volume preserving methods for split systems with a special structure

5. From conditions for vector fields to conditions for integrators
From integrators to vector fields and vice-versa

**BACKWARD ERROR ANALYSIS**

\[ \dot{y} = f(y) \]

\[ \dot{z} = f_h(z) \]

numerical method

exact solution

\[ y_0, y_1, y_2, y_3, \ldots \]

\[ z(0), z(h), z(2h), \ldots \]

Back to the black forest

Though what follows is valid for multicoloured trees, for simplicity we now turn back to the monocolour situation.
Substitution law

From partitions and skeletons to the formula

Definition
Given a partition $p$ of $t$, the corresponding skeleton $\chi_p$ is the tree obtained by contracting each tree of $p$ to a single vertex and by re-establishing the cut edges.

Table: The 8 partitions of a tree of order 4 with associated skeleton and forest

<table>
<thead>
<tr>
<th>$p$</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\chi_p$</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
</tr>
<tr>
<td>$v_p$</td>
<td>Y</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
<td>·</td>
</tr>
</tbody>
</table>
For \( b(\emptyset) = 0 \), the vector field \( h^{-1} B_f(b, y) \) inserted into \( B_g(a, y) \), i.e. with \( g = h^{-1} B_f(b, y) \) gives a B-series

\[
B_g(a, y) = B_f(b \star a, y).
\]

We have \((b \star a)(\emptyset) = a(\emptyset)\) and for all \( t \in T \),

\[
(b \star a)(t) = \sum_{p \in \mathcal{P}(t)} a(\chi_p) b(v_p).
\]
**Substitution law**

<table>
<thead>
<tr>
<th>Table: Substitution law $\star$ for the first trees.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(b \star a)(\emptyset) = a(\emptyset)$</td>
</tr>
<tr>
<td>$(b \star a)(\cdot) = a(\cdot)b(\cdot)$</td>
</tr>
<tr>
<td>$(b \star a)(\bullet) = a(\cdot)b(\bullet) + a(\bullet)b(\cdot)^2$</td>
</tr>
<tr>
<td>$(b \star a)(\bigtriangledown) = a(\cdot)b(\bigtriangledown) + 2a(\bullet)b(\cdot)b(\bullet) + a(\bigtriangledown)b(\cdot)^3$</td>
</tr>
<tr>
<td>$(b \star a)(\bigcirc) = a(\cdot)b(\bigcirc) + 2a(\bullet)b(\cdot)b(\bullet) + a(\bigcirc)b(\cdot)^3$</td>
</tr>
</tbody>
</table>

**Remark**

This law *essentially* coincides with the convolution product in the Hopf algebra of Calaque, Ebrahimi-Fard and Manchon.
Let $\omega$ denote the inverse element of $\frac{1}{\gamma} - \delta_0$ for $\star$. The **backward error** coefficients $b$ can be computed as follows:

**Backward error character** $\omega$

$$\forall t \in \mathcal{T}, \ b(t) = ((a - \delta_0) \star \omega)(t).$$

**Lemma**

*The coefficients $\omega$ satisfy the following relation for all $m$-uplets, $m \geq 2$, of trees $(u_1, \ldots, u_m) \in \mathcal{T}^m$:

$$\sum_{I \cup J = \{1, \ldots, m\}, \ I \cap J = \emptyset} \omega\left(\times_{i \in I} u_i \circ \prod_{j \in J} u_j\right) = 0,$$

with the conventions $u \circ \emptyset = u$ and $\emptyset \circ u = \emptyset.$*
From 1-cuts to multicuts

Let \( a \in \text{Alg}(\mathcal{H}, \mathbb{R}) \) and \( b \in \text{VF}(\mathcal{H}, \mathbb{R}) \). Then one has

\[
\forall o = (t_1 \ldots t_m) \in AT, \quad \sum_{t \in C(o)} b(t) = 0 \iff \forall o = (t_1 \ldots t_m) \in AT, \quad \sum_{k=1}^{m} (-1)^{k+1} \sum_{t \in C_k(o)} a(u) = 0.
\]
Consider the case $m = 3$, and, for instance, $o = (t_1 t_2 t_3)$. We have to compute

$$b(t_1 \circ t_2 \circ t_3) + b(t_2 \circ t_3 \circ t_1) + b(t_3 \circ t_1 \circ t_2)$$

in terms of the $a$'s. Given $(p_1, p_2, p_3)$ in $\mathcal{P}(t_1) \times \mathcal{P}(t_2) \times \mathcal{P}(t_3)$, a partition $p \in \mathcal{P}(t_1 \circ t_2 \circ t_3)$ is of the form

<table>
<thead>
<tr>
<th>$p$</th>
<th>$p_1 \circ p_2 \circ p_3$</th>
<th>$p_1 \circ p_2 \circ p_3$</th>
<th>$p_1 \circ p_2 \circ p_3$</th>
<th>$p_1 \circ p_2 \circ p_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_p$</td>
<td>$x_{p_1} \times x_{p_2} \times x_{p_3}$</td>
<td>$x_{p_1} \times x_{p_2} \circ x_{p_3}$</td>
<td>$x_{p_1} \circ x_{p_2} \times x_{p_3}$</td>
<td>$x_{p_1} \circ x_{p_2} \circ x_{p_3}$</td>
</tr>
<tr>
<td>$v_p$</td>
<td>$v_{p_1} v_{p_2} v_{p_3} r_{p_1} \circ r_{p_2} \circ r_{p_3}$</td>
<td>$v_{p_1} v_{p_2} v_{p_3} (r_{p_1} \circ r_{p_2}) r_{p_3}$</td>
<td>$v_{p_1} v_{p_2} v_{p_3} (r_{p_2} \circ r_{p_3}) r_{p_3}$</td>
<td>$v_{p_1} v_{p_2} v_{p_3} r_{p_1} r_{p_2} r_{p_3}$</td>
</tr>
</tbody>
</table>

**Table:** Terms in the substitution law for $t_1 \circ t_2 \circ t_3$
Hence,

\[ b(t_1 \circ t_2 \circ t_3) = \sum_{(p_1, p_2, p_3)} a(v^*_p, v^*_p, v^*_p) \times \]

\[ \left( \omega(\chi_{p_1} \times \chi_{p_2} \times \chi_{p_3})a(r_{p_1} \circ r_{p_2} \circ r_{p_3}) \right. \]

\[ + \omega(\chi_{p_1} \times \chi_{p_2} \circ \chi_{p_3})a(r_{p_1} \circ r_{p_2})a(r_{p_3}) \]

\[ + \omega(\chi_{p_1} \circ \chi_{p_2} \times \chi_{p_3})a(r_{p_1})a(r_{p_2} \circ r_{p_3}) \]

\[ + \omega(\chi_{p_1} \circ \chi_{p_2} \circ \chi_{p_3})a(r_{p_1})a(r_{p_2})a(r_{p_3}) \]

1-cut term

2-cut term

2-cut term

3-cut term
For $b(t_1 \circ t_2 \circ t_3) + b(t_2 \circ t_3 \circ t_1) + b(t_3 \circ t_1 \circ t_2)$ we get:

1-cut terms

$$\omega(\chi_{p_1} \times \chi_{p_2} \times \chi_{p_3}) \left( a(r_{p_1} \circ r_{p_2} \circ r_{p_3}) + a(r_{p_2} \circ r_{p_3} \circ r_{p_1}) + a(r_{p_3} \circ r_{p_1} \circ r_{p_2}) \right).$$

2-cut terms

$$a(r_{p_3})a(r_{p_1} \circ r_{p_2})\left( \omega(\chi_{p_1} \times \chi_{p_2} \circ \chi_{p_3}) + \omega(\chi_{p_3} \circ \chi_{p_1} \times \chi_{p_2}) \right) + \ldots$$

where

$$\omega(\chi_{p_1} \times \chi_{p_2} \circ \chi_{p_3}) + \omega(\chi_{p_3} \circ \chi_{p_1} \times \chi_{p_2}) = -\omega(\chi_{p_1} \times \chi_{p_2} \times \chi_{p_3}).$$

3-cut terms

$$a(r_{p_1})a(r_{p_2})a(r_{p_3})\left( \omega(\chi_{p_1} \circ \chi_{p_2} \circ \chi_{p_3}) + \omega(\chi_{p_2} \circ \chi_{p_3} \circ \chi_{p_1}) + \omega(\chi_{p_3} \circ \chi_{p_1} \circ \chi_{p_2}) \right)$$

i.e.,

$$a(r_{p_1})a(r_{p_2})a(r_{p_3})\omega(\chi_{p_1} \times \chi_{p_2} \times \chi_{p_3}).$$
The character $\omega$ and its role