Preserving invariants and volume for split systems

Philippe Chartier[1] Ander Murua[2]

[1]IPSO
INRIA-Rennes and ENS Cachan, Antenne de Bretagne

[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 stru
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 stru
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

$\frac{d}{dt}H(p,q) = \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial q}\dot{q} = 0 \; hence \; H(p,q) = Const$

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

$\sum_{i=1}^{N} p_i = Const$ and $\sum_{i=1}^{N} q_i \times p_i = Const$

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

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

Theorem

$\frac{d}{dt}(y_1 + y_2 + y_3) = 0$ *hence* $I(y) = y_1 + y_2 + y_2 = Const.$

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
- Conservation of the spectrum by matrix flows

Isospectral matrix equations

$$\dot{L} \quad = \quad B(L)\,L - L\,B(L) \text{ with } B(L) \text{ skew-symmetric.}$$

Theorem

Let $\dot{U} = B(L(t))U$, $U(0) = I$. *Then,* $L(t) = U(t)L_0U(t)^{-1}$.

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

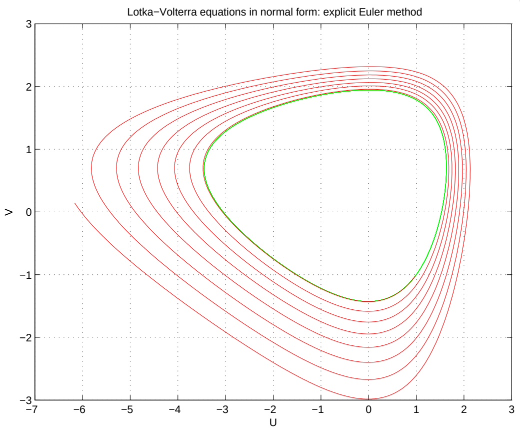
$$\dot{y} \quad = \quad f(y) \text{ with } \mathrm{div}(f) = 0.$$

Theorem

The flow φ_t preserves the volume, i.e. $\int_{\varphi_t(A)} dy = \int_A dy$.

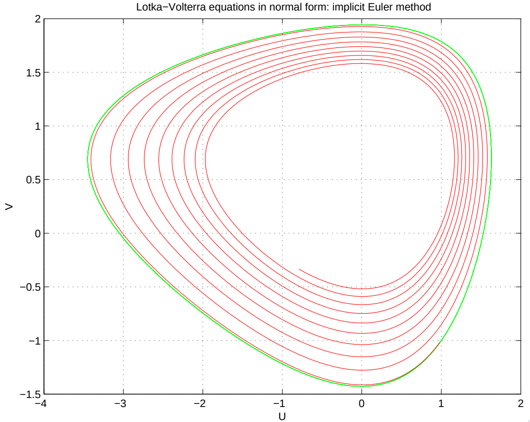
A prey-predator model in normal form

$$\begin{aligned}\dot{U} &= e^{V} - 2 = f(V)\\ \dot{V} &= 1 - e^{U} = g(U)\end{aligned}$$



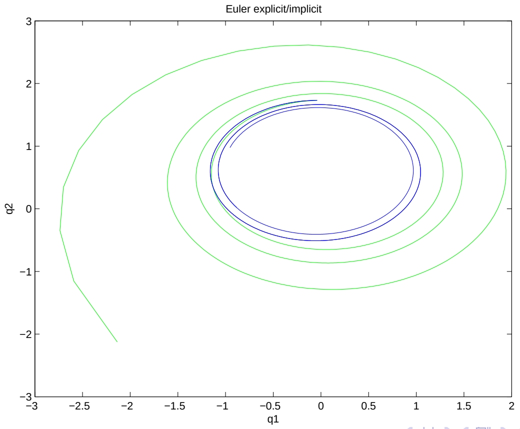
A prey-predator model in normal form

$$\dot{U} = e^V - 2 = f(V)$$
$$\dot{V} = 1 - e^U = g(U)$$



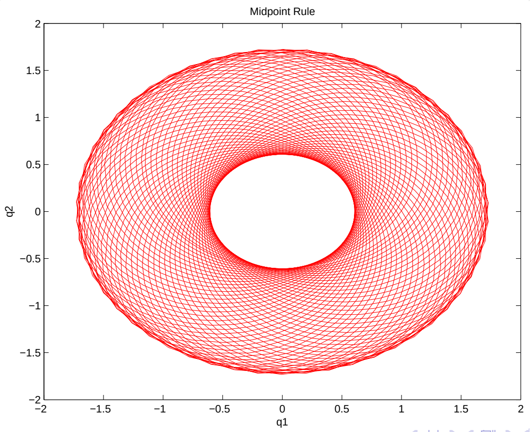
2-D Kepler Problem

$$H(p,q) = \frac{1}{2}p^T p - \frac{1}{\sqrt{q^T q}} = T(p) + V(q) \Longleftrightarrow \ddot{q} = -V'(q).$$



2-D Kepler Problem

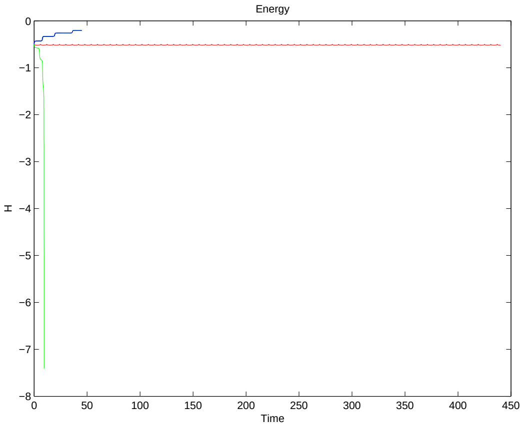
$$H(p,q) = \frac{1}{2}p^T p - \frac{1}{\sqrt{q^T q}} = T(p) + V(q) \iff \ddot{q} = -V'(q).$$



Improved qualitative behavior of *geometric* integrators

2-D Kepler Problem

$$H(p,q) = \frac{1}{2}p^T p - \frac{1}{\sqrt{q^T q}} = T(p) + V(q) \Longleftrightarrow \ddot{q} = -V'(q).$$



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 stru
5. From conditions for vector fields to conditions for integrators

The two classes of problems considered

We consider systems of ODEs of the form

Split vector fields systems

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

such that each individual vector field has the invariant function I

Common Invariant

$$0 = (\nabla_y I(y))^T f^{[\nu]}(y), \quad \nu = 1, \ldots, N,$$

The two classes of problems considered

We consider systems of ODEs of the form

Split vector fields systems

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

or preserves the volume form

Divergence-free

$$0 \quad = \quad \operatorname{div} f^{[\nu]}(y), \qquad \nu = 1, \ldots, N$$

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 Φ_h^f at time $t+h$.

The modified vector field

associated to a numerical integrator Φ_h^f 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 $\Phi_h^f(y)$.

Invariant-preserving integrators(1)

Φ_h^f preserves I if $I\left(\Phi_h^f(y)\right) = I(y)$ for any y.

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 Φ_h^f at time $t+h$.

The modified vector field

associated to a numerical integrator Φ_h^f 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 $\Phi_h^f(y)$.

Invariant-preserving integrators(2)

Φ_h^f preserves I if $\left(\nabla I(y)\right)^T \tilde{f}_h(y) = 0$ 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 $\Phi_h^f(y)$ at time $t + h$.

The modified vector field

associated to a numerical integrator Φ_h^f 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 $\Phi_h^f(y)$.

Volume-preserving integrators(1)

Φ_h^f preserves the volume if $\det\left(\frac{\partial \Phi_h^f(y)}{\partial y}\right) = 1$ 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 $\Phi_h^f(y)$ at time $t+h$.

The modified vector field

associated to a numerical integrator Φ_h^f 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 $\Phi_h^f(y)$.

Volume-preserving integrators(2)

Φ_h^f preserves the volume if $\mathrm{div}\left(\tilde{f}_h(y)\right) = 0$ 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 $\Phi_h^f(y)$ at time $t+h$.

The modified vector field

associated to a numerical integrator Φ_h^f 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 $\Phi_h^f(y)$.

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

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

$B_1^+(\bullet \circ) = \left[\bullet \circ\right]_1 =$  and $B_2^+(\bullet \bullet) = \left[\bullet \bullet\right]_2 =$ 

$B^-($  $) = \bullet \bullet \bullet$ and $B^-($  $) =$ 

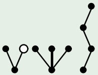
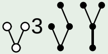
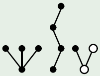
Order and symmetry

Definition

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

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

Example

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

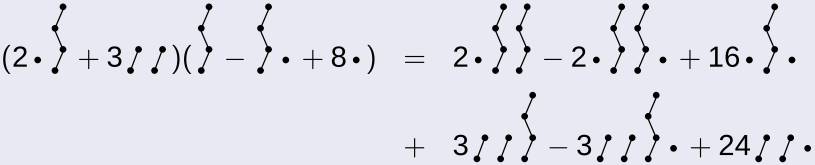
Structure (Connes and Kreimer 98, Brouder 04)

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 $uv = vu$),
- $\forall u \in \mathcal{F},\ u\,e = e\,u = u$.

Calculus in $\mathcal{H}$



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 $(\lambda, \mu) \in \mathbb{R}^2$:

$$\begin{aligned}(\lambda u + \mu v) \otimes w &= \lambda(u \otimes w) + \mu(v \otimes w),\\ w \otimes (\lambda u + \mu v) &= \lambda(w \otimes u) + \mu(w \otimes v),\\ (u \otimes v)(w \otimes x) &= (uw \otimes vx).\end{aligned}$$

Definition

The co-product Δ 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. $\forall u = t_1 \dots t_n \in \mathcal{F},\ \Delta(u) = \Delta(t_1) \dots \Delta(t_n)$.

The co-product

Example

$\Delta($  $)$ $=$  $\otimes e + (id \otimes B_2^+)\Delta(\bullet\circ)$

$=$  $\otimes e + (id \otimes B_2^+)\Delta(\bullet)\Delta(\circ)$

$=$  $\otimes e + (id \otimes B_2^+)(\bullet \otimes e + e \otimes \bullet)(\circ \otimes e + e \otimes \circ)$

$=$  $\otimes e$

$+(id \otimes B_2^+)\left(\bullet\circ \otimes e + \bullet \otimes \circ + \circ \otimes \bullet + e \otimes \bullet\circ\right)$

$=$  $\otimes e + \bullet\circ \otimes \circ + \bullet \otimes$  $+ \circ \otimes$  $+ e \otimes$ 

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

Example

$F($  $) = \left(f^{[1]}\right)' f^{[2]}$

$F($  $) = \left(f^{[2]}\right)''(y)\left(f^{[1]}, f^{[2]}\right)$

$F($  $) = \left(f^{[1]}\right)' \left(f^{[2]}\right)' f^{[1]}$

Elementary differential operators

Definition

Let $u = t_1 \dots t_k$ 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:

$$\begin{aligned} X(u) : \mathcal{D} &\rightarrow \mathcal{D} \\ g &\mapsto X(u)[g] = g^{(k)}\Big(F(t_1), \dots, F(t_k)\Big). \end{aligned}$$

Example

$$\begin{aligned} X(e)[g] &= g \\ X(\bullet)[g] &= g' f^{[1]} \\ X(\overset{\circ}{\bullet})[g] &= g' \left(f^{[1]}\right)' f^{[2]} \\ X(\overset{\bullet}{\bullet} \circ \bullet)[g] &= g^{(3)}\Big(\left(f^{[1]}\right)' f^{[1]}, f^{[2]}, f^{[1]}\Big) \end{aligned}$$

B-series and S-series

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

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

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

Example (Implicit/Explicit Euler)

$$\begin{aligned} y_1 &= y_0 + h\left(f^{[1]}(y_1) + f^{[2]}(y_0)\right) \\ &= y_0 + hF(\bullet)(y_0) + hF(\circ)(y_0) + h^2F(\bullet\!-\!\bullet)(y_0) + h^2F(\bullet\!-\!\circ)(y_0) \\ &\quad + \ldots \end{aligned}$$

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

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

Example (Implicit/Explicit Euler)

$$\begin{aligned} g(y_1) &= g\left(y_0 + hf^{[1]}(y_1) + hf^{[2]}(y_0)\right) \\ &= X(e)[g] + h(X(\bullet)[g] + X(\circ)[g]) + h^2(X([\bullet]_\bullet)[g] + X([\circ]_\bullet)[g]) \\ &\quad + \frac{h^2}{2}\left(X(\bullet^2)[g] + 2X(\bullet\circ)[g] + X(\circ^2)[g]\right) + \dots \end{aligned}$$

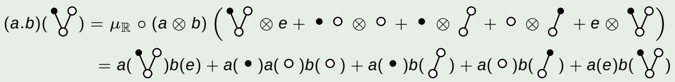
Composition of series and co-product in $\mathcal{H}$

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 $B(a.b,y)$, with coefficients a.b defined on $\mathcal{T}$ by

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

Example



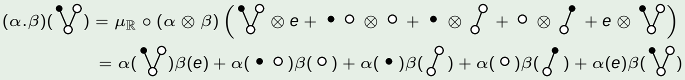
Composition of series and co-product in $\mathcal{H}$

Theorem (Composition of S-series)

Let α and β 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 $\alpha.\beta$ 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



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 stru
5. From conditions for vector fields to conditions for integrators

The action of a function I on a B-series

It can be viewed as S-series:

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

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

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

i.e.

$$\boxed{S(\alpha)[I] = I,}$$

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

The annihilating left ideal $\mathcal{I}[I]$ of I

Using the assumption of a common invariant I

For $\nu = 1, \ldots, N$, $X(\bullet_\nu)[I] = (\nabla I) f^{[\nu]} = 0$. Hence,

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

Lemma

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

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

Integrators preserving general invariants

Theorem

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

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

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

Theorem

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

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

For quadratic

first integral I, the condition becomes

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

while for cubic invariants I, one needs in addition that

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

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 stru
5. From conditions for vector fields to conditions for integrators

Split systems with zero-divergence

Divergence-free B-series

For systems of the form

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

a B-series modified vector field is divergence free if

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

Question

How to compute and represent the terms in $\mathrm{div}(F(t)(y))$?

A convenient formula for the derivative of an elementary differential

Notation

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

The formula

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

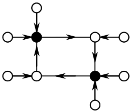
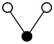
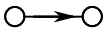
The grafting operation is meant to operate from right to left.

$$\frac{\mathrm{div}(F(t))}{\sigma(t)} = \frac{Tr\left(F^*(t)\right)}{\sigma(t)} + \sum_{t_1 \circ t_2 \circ \cdots \circ t_m = t} \frac{Tr\left(F^*(t_1) \ldots F^*(t_m)\right)}{\sigma(t_1) \ldots \sigma(t_m)}.$$

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 $\mathcal{AT}_n$.

$o =$  $= (t_1 t_2 t_1 t_2)$ $\quad t_1 =$  $=$ , $\quad t_2 =$  $=$ .

1-cuts of aromatic trees

Definition

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

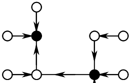
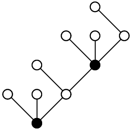
$$C(o) = \{s_1, \dots, s_m\}. \tag{1}$$

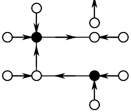
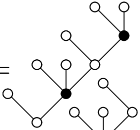
Now, let π_m be the circular permutation of $\{1, \dots, m\}$ and let θ be

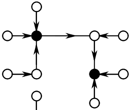
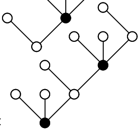
$$\theta = \#\Big\{ l \in \{0, \dots, m-1\} : \quad (t_{\pi_m^l(1)}, \dots, t_{\pi_m^l(m)}) = (t_1, \dots, t_m) \Big\},$$

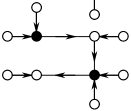
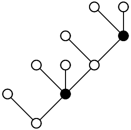
so that, for each i, there are θ copies of s_i in the list $C(o)$. Then the symmetry coefficient of o is defined as $\sigma(o) = \theta \prod_i \sigma(t_i)$.

The list $C(o) = \{s_1, s_2, s_3, s_4\}$ for $o = (t_1 t_2 t_1 t_2)$

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

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

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

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

Divergence of a B-series vector field

Definition (Elementary divergence)

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

$$\boxed{\mathrm{div}(o) \quad = \quad Tr\Big(F^*(t_1)\dots F^*(t_m)\Big).}$$

Collecting the terms

$$\begin{aligned}\mathrm{div}\big(B(b)\big) &= \sum_{t\in\mathcal{T}} b(t)h^{|t|} \sum_{m\geq 2} \sum_{t_1\circ\cdots\circ t_m=t} \frac{\mathrm{div}\big((t_1\dots t_m)\big)}{\sigma(t_1)\cdots\sigma(t_m)} \\ &= \sum_{n\geq 2} h^n \sum_{o\in\mathcal{AT}_n} \Big(\sum_{t\in C(o)} b(t)\Big)\frac{\mathrm{div}(o)}{\sigma(o)}.\end{aligned}$$

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:

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

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

$$\begin{aligned} 0 &= b(t_1 \circ t_2 \circ t_3) + b(t_2 \circ t_1 \circ t_3) + b(t_3 \circ t_2 \circ t_1), \\ &= b(t_1 \circ (t_2 \circ t_3)) + b(t_2 \circ (t_1 \circ t_3)) + b(t_3 \circ (t_2 \circ t_1)), \\ &= -b((t_2 \circ t_3) \circ t_1) - b((t_1 \circ t_3) \circ t_2) - b((t_2 \circ t_1) \circ t_3), \\ &= -b(t_2 \circ t_1 t_3) - b(t_1 \circ t_2 t_3) - b(t_2 \circ t_1 t_3). \end{aligned}$$

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

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 $u = [v_1, \ldots, v_m]_\bullet$, 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

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

White trees

For $v = [w_1, \ldots, w_n]_\circ$, 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

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

Consequence

$$\mathrm{div}(o) \neq 0 \text{ iff } o = (u_1 v_1 w_1 u_2 v_2 w_2 \ldots u_m v_m w_m), \; m \geq 1.$$

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*

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

Example

An implicit "non-symplectic" RK-method

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

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

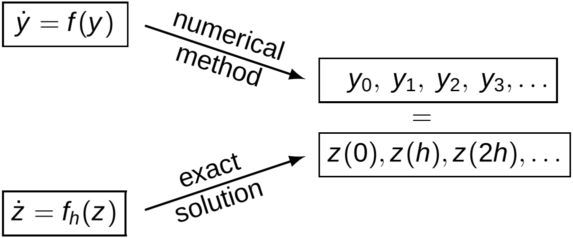
3 **Conditions for invariants-preservation**
- Numerical methods preserving invariants
- The case of quadratic and cubic invariants
- B-series methods preserving all cubic invariants

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 stru

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

From integrators to vector fields and vice-versa

BACKWARD ERROR ANALYSIS



Back to the black forest

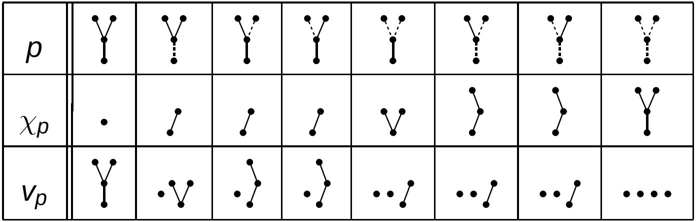
Though what follows is valid for multicoloured trees, for simplicity we now turn back to the monocolour situation.

From partitions and skeletons to the formula

Definition

Given a partition p of t, the corresponding *skeleton* χ_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



Theorem

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 $t \in \mathcal{T}$,

$$(b \star a)(t) = \sum_{p \in \mathcal{P}(t)} a(\chi_p) b(v_p).$$

Table: Substitution law $\star$ for the first trees.

$$
\begin{aligned}
(b\star a)(\emptyset) &= a(\emptyset)\\
(b\star a)(\bullet) &= a(\bullet)b(\bullet)\\
(b\star a)([\bullet]) &= a(\bullet)b([\bullet]) + a([\bullet])b(\bullet)^2\\
(b\star a)([\bullet\bullet]) &= a(\bullet)b([\bullet\bullet]) + 2a([\bullet])b(\bullet)b([\bullet]) + a([\bullet\bullet])b(\bullet)^3\\
(b\star a)([[\bullet]]) &= a(\bullet)b([[\bullet]]) + 2a([\bullet])b(\bullet)b([\bullet]) + a([[\bullet]])b(\bullet)^3
\end{aligned}
$$

Remark

This law *essentially* coincides with the convolution product in the Hopf algebra of Calaque, Ebrahimi-Fard and Manchon.

Let ω denote the inverse element of $\frac{1}{\gamma} - \delta_\emptyset$ for $\star$. The **backward error** coefficients b can be computed as follows:

Backward error character ω

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

Lemma

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

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

with the conventions $u \circ \emptyset = u$ and $\emptyset \circ u = \emptyset$.

From 1-cuts to multicuts

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

$$\forall o = (t_1 \dots t_m) \in \mathcal{AT}, \sum_{t \in C(o)} b(t) = 0 \text{ iff}$$

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

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: Terms in the substitution law for $t_1 \circ t_2 \circ t_3$

p	$p_1 \circ p_2 \circ p_3$	$p_1 \circ p_2 \diamond p_3$	$p_1 \diamond p_2 \circ p_3$	$p_1 \diamond p_2 \diamond p_3$
χp	$\chi p_1 \times \chi p_2 \times \chi p_3$	$\chi p_1 \times \chi p_2 \circ \chi p_3$	$\chi p_1 \circ \chi p_2 \times \chi p_3$	$\chi p_1 \circ \chi p_2 \circ \chi p_3$
v_p	$v^*_{p_1} v^*_{p_2} v^*_{p_3} r_{p_1} \circ r_{p_2} \circ r_{p_3}$	$v^*_{p_1} v^*_{p_2} v^*_{p_3} (r_{p_1} \circ r_{p_2}) r_{p_3}$	$v^*_{p_1} v^*_{p_2} v^*_{p_3} r_{p_1} (r_{p_2} \circ r_{p_3})$	$v^*_{p_1} v^*_{p_2} v^*_{p_3} r_{p_1} r_{p_2} r_{p_3}$

Hence,

$$b(t_1 \circ t_2 \circ t_3) = \sum_{(p_1,p_2,p_3)} a(v_{p_1}^* v_{p_2}^* v_{p_3}^*) \times$$

$$\Big(\omega(\chi_{p_1} \times \chi_{p_2} \times \chi_{p_3}) a(r_{p_1} \circ r_{p_2} \circ r_{p_3}) \quad \text{1-cut term}$$
$$+\omega(\chi_{p_1} \times \chi_{p_2} \circ \chi_{p_3}) a(r_{p_1} \circ r_{p_2}) a(r_{p_3}) \quad \text{2-cut term}$$
$$+\omega(\chi_{p_1} \circ \chi_{p_2} \times \chi_{p_3}) a(r_{p_1}) a(r_{p_2} \circ r_{p_3}) \quad \text{2-cut term}$$
$$+\omega(\chi_{p_1} \circ \chi_{p_2} \circ \chi_{p_3}) a(r_{p_1}) a(r_{p_2}) a(r_{p_3}) \quad \text{3-cut term} \Big)$$

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

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

2-cut terms

$$a(r_{p_3})a(r_{p_1} \circ r_{p_2})\Big(\omega(\chi_{p_1} \times \chi_{p_2} \circ \chi_{p_3}) + \omega(\chi_{p_3} \circ \chi_{p_1} \times \chi_{p_2})\Big) + \dots$$

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

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

i.e., $a(r_{p_1})a(r_{p_2})a(r_{p_3})\omega(\chi_{p_1} \times \chi_{p_2} \times \chi_{p_3})$.

THIS IS THE END