Invariant preserving integrators :

An algebraic approach

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With the contributions of E. Faou, E. Hairer, A. Murua and

G. Vilmart for some of the recent results

Qualitative properties of $\dot{y} = f(y)$

There are many situations where the differential system has structural properties that owed to be preserved :

1. First integral : $\frac{d}{dt} I(y) = 0$.
2. Symplectic structure (Hamiltonian systems : $f(y) = J^{-1} \nabla H(y)$).
3. Symmetry : $\rho(f(y)) = -f(\rho(y))$.

Trajectories of 2-D Kepler with various methods

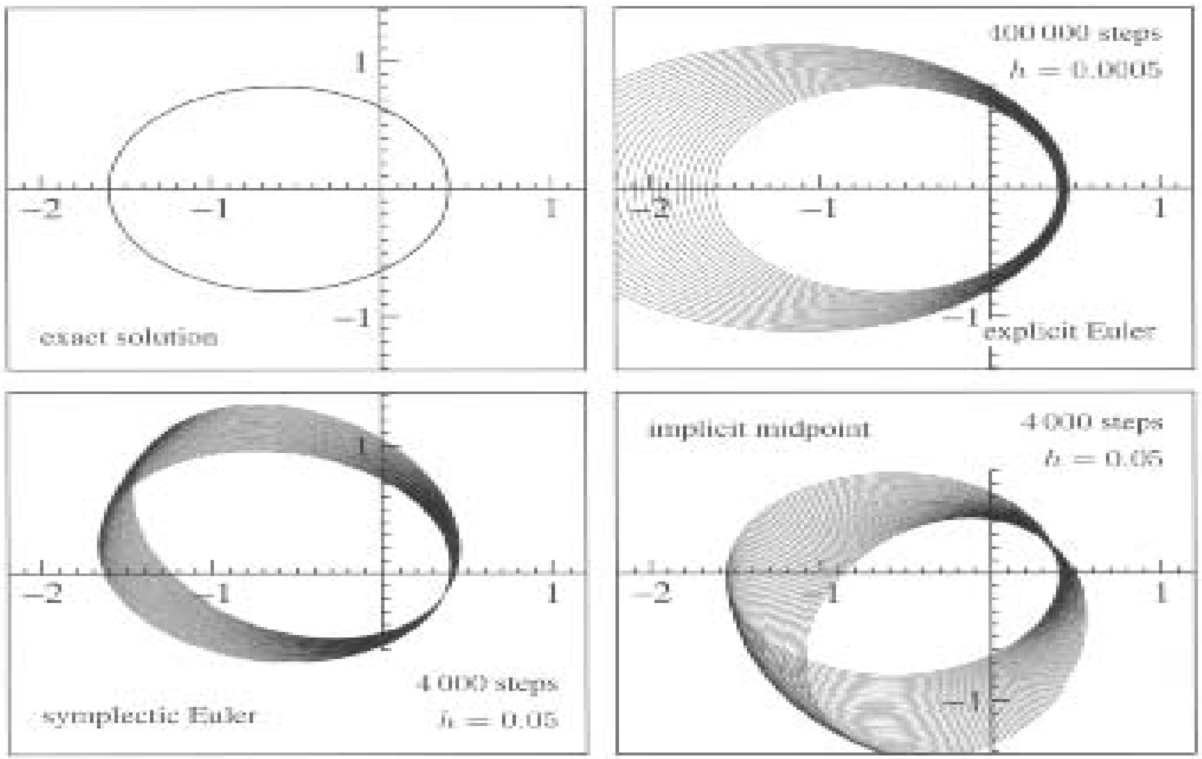


FIG. 1 – E. Hairer, Geometric Integration, pp. 5

Energy conservation - Global Error

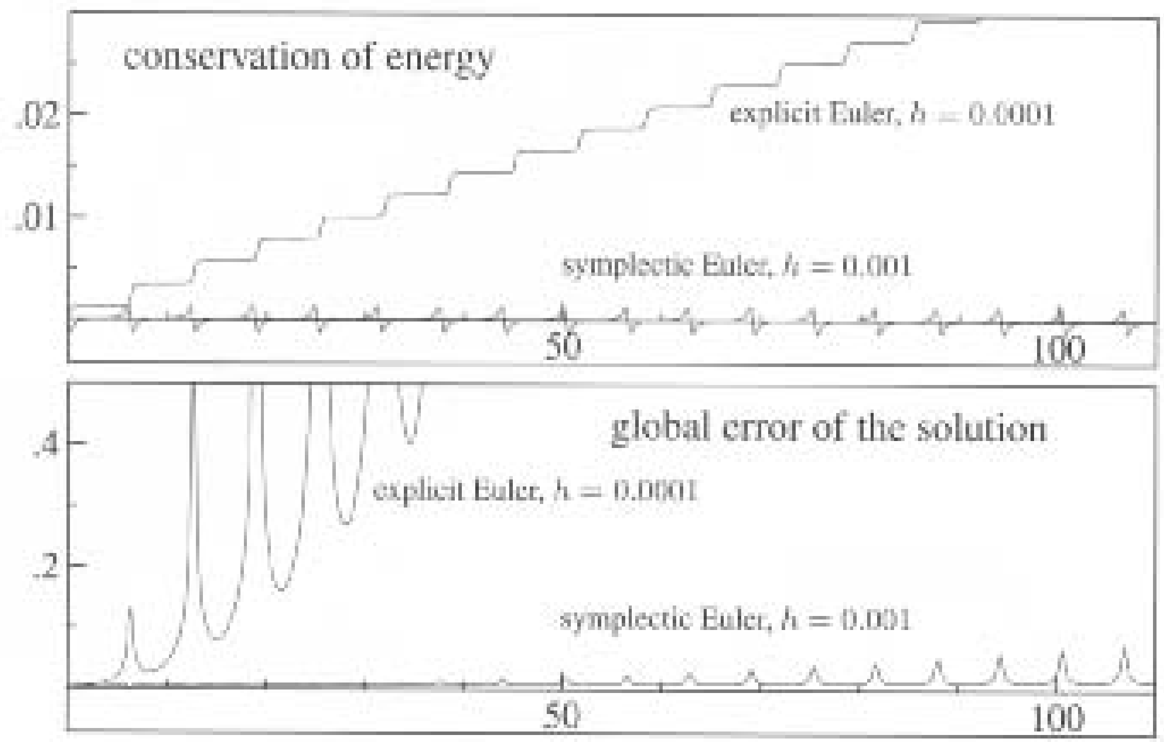


FIG. 2 – E. Hairer, Geometric Integration, pp. 6

Geometric numerical integration

The main objective of GNI is to study existing numerical integrators and design new ones that preserve some or all of these properties, with applications to

– celestial mechanics,

– robotics,

– molecular simulation...,

where obtaining an accurate approximation over long integration intervals is out of reach.

The main idea of GNI is to re-interpret the numerical method as the exact solution of a modified equation whose qualitative features can be described.

Modified equations

modified problem $\begin{cases} \dot{\hat{y}} = \hat{f}(\hat{y}) \\ \hat{y}(0) = y_0 \end{cases}$

$\searrow$ exact solution : $\hat{y}(nh) = y_n$

$$y_{n+1} = \Phi_h^f(y_n)$$

$\nearrow$ numerical solution : $y_n \approx y(nh)$

initial problem $\begin{cases} \dot{y} = f(y) \\ y(0) = y_0 \end{cases}$

Strictly speaking, this diagram holds true only formally : its validity can be justified by a rigorous study of error terms (optimal truncature of the series involved leads to exponentially small errors).

Taylor expansions or the urgent necessity of trees

In trying to get the Taylor expansion of the implicit Euler solution

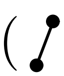
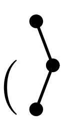
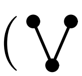
$$y_1 \quad = \quad y_0 + hf(y_1)$$

one gets successively (where we have omitted the argument y_0 in f, f', ...)

$$y_1 \quad = \quad y_0 + h\underbrace{f}_{=y'} + \mathcal{O}(h^2),$$

$$y_1 \quad = \quad y_0 + h\underbrace{f}_{=y'} + h^2\underbrace{f'f}_{=y''} + \mathcal{O}(h^3),$$

$$y_1 \quad = \quad y_0 + h\underbrace{f}_{=y'} + h^2\underbrace{f'f}_{=y''} + h^3\Big(\underbrace{f'f'f + \frac{1}{2}f''(f,f)}_{\neq y^{(3)} = f'f'f + f''(f,f)}\Big) + \mathcal{O}(h^4),$$

$= \quad y_0 + hF(\bullet) + h^2F($  $) + h^3(F($  $) + \frac{1}{2}F($  $)) + \ldots$

PART I : formal numerical integrators

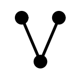
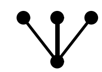
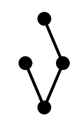
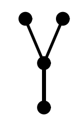
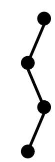
Rooted trees

Definition 1 (Rooted trees) *The set of rooted trees is recursively defined by :*

1. $\bullet \in \mathcal{T}$
2. $(t_1, \ldots, t_n) \in \mathcal{T}^n \Rightarrow t = [t_1, \ldots, t_n] \in \mathcal{T}$

The order of a tree $|t|$ *is its number of vertices.*

Examples of rooted trees

Arbre t								
Ordre $\vert t\vert$	1	2	3	3	4	4	4	4
Symétrie $\sigma(t)$	1	1	2	1	6	1	2	1

TAB. 1 – Rooted trees of orders 1 to 4

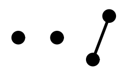
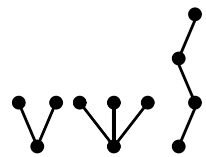
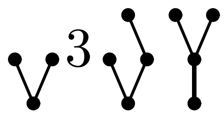
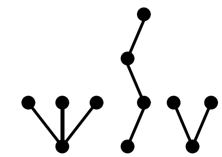
Forests (monomials of rooted trees)

Definition 2 (Forest) *A forest u is an unordered k-uplet of trees. If $u = t_1 \ldots t_1 t_2 \ldots t_2 \ldots t_n \ldots t_n$ where the trees t_i's are all distinct where each t_i is repeated r_i times, than the order and the symmetry of u are recursively defined by :*

1. $|u| = \sum_{i=1}^{n} r_i |t_i|$,
2. $\sigma(u) = \prod_{i=1}^{n} r_i! \sigma(t_i))^{r_i}$.

We denote by e the empty forest and by $\mathcal{F}$ the set forests.

Examples of forests

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

TAB. 2 – A few forests

The algebra of forests

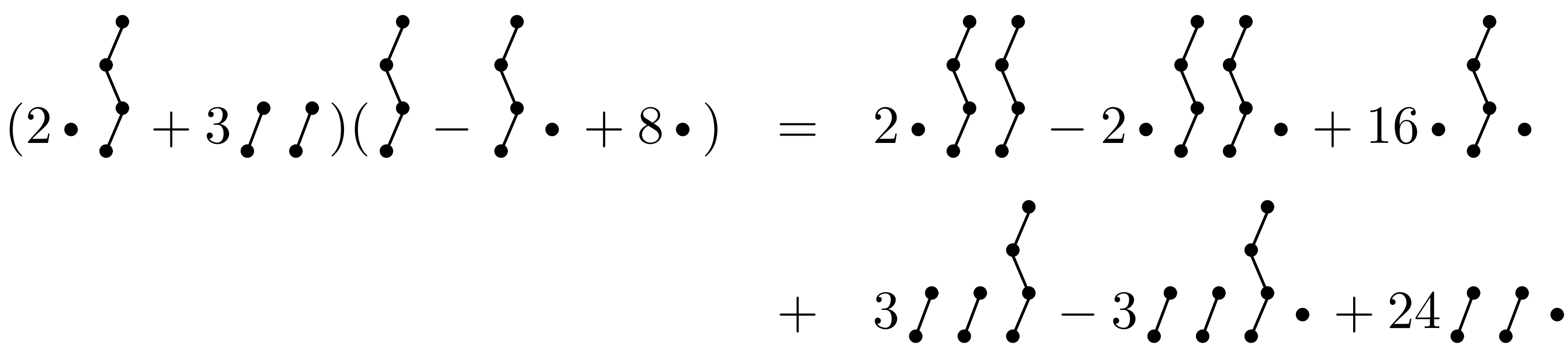
The set $\mathcal{F}$ can be naturally endowed with an algebra structure $\mathcal{H}$ on $\mathbb{R}$:

– $\forall\,(u,v) \in \mathcal{F}^2, \forall\,(\lambda,\mu) \in \mathbb{R}^2, \lambda u + \mu v \in \mathcal{H}$,

– $\forall\,(u,v) \in \mathcal{F}^2,\; u\,v \in \mathcal{H}$, where $u\,v$ denotes the commutative product of the forests u and v,

– $\forall\,u \in \mathcal{F},\; u\,e = e\,u = u$, where e is the empty forest.

<u>Example of calculus in $\mathcal{H}$:</u>



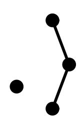
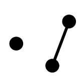
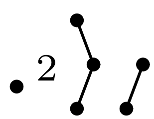
The tensor product of $\mathcal{H}$ by itself

Definition 3 *The tensor product of $\mathcal{H}$ with itself is the set of elements of the form $u \otimes v$ with u and v in $\mathcal{H}$, such that :*

- $\forall\,(u, v, w) \in \mathcal{H}^3,\ (u + v) \otimes w = u \otimes w + v \otimes w,$
- $\forall\,(u, v, w) \in \mathcal{H}^3,\ u \otimes (v + w) = u \otimes v + u \otimes w,$
- $\forall\,(u, v) \in \mathcal{H}^2, \forall\,\lambda \in \mathbb{R},\ \lambda \cdot u \otimes v = (\lambda \cdot u) \otimes v = u \otimes (\lambda \cdot v).$

The product on $\mathcal{H}$ can be viewed as a mapping m from $\mathcal{H} \otimes \mathcal{H}$ into $\mathcal{H}$:

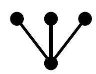
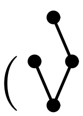
$$\forall\,(u, v) \in \mathcal{H}^2,\ u\,v = m(u \otimes v).$$

Example : $m($  $\otimes$  $) =$ 

The co-product

We define the operators B^+ and B^- by :

$$\begin{array}{rcl} B^+ : \mathcal{H} & \to & \mathcal{T} \\ u = t_1 \ldots t_n & \mapsto & [t_1, \ldots, t_n] \end{array} \qquad \begin{array}{rcl} B^- : \mathcal{T} & \to & \mathcal{H} \\ t = [t_1, \ldots, t_n] & \mapsto & t_1 \ldots t_n \end{array}$$

Examples : $B^+(\bullet \bullet \bullet) = \left[\bullet \bullet \bullet \right] =$  et $B^-($  $) = \bullet$ 

Definition 4 (Co-product) *The co-product Δ is a morphism from $\mathcal{H}$ to $\mathcal{H} \otimes \mathcal{H}$ defined recursively by :*

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

Examples of co-products

$$
\begin{aligned}
\Delta(\bullet) &= \bullet \otimes e + e \otimes \bullet, \\
\Delta(\overset{\bullet}{\underset{\bullet}{|}}) &= \overset{\bullet}{\underset{\bullet}{|}} \otimes e + (id_{\mathcal{H}} \otimes B^{+}) \circ \Delta(\bullet) \\
&= \overset{\bullet}{\underset{\bullet}{|}} \otimes e + (id_{\mathcal{H}} \otimes B^{+})(\bullet \otimes e + e \otimes \bullet) \\
&= \overset{\bullet}{\underset{\bullet}{|}} \otimes e + e \otimes \overset{\bullet}{\underset{\bullet}{|}} + \bullet \otimes \bullet, \\
\Delta(\bullet\,\bullet) &= \Delta(\bullet)\Delta(\bullet) = (e \otimes \bullet + \bullet \otimes e)(e \otimes \bullet + \bullet \otimes e), \\
&= e \otimes \bullet\,\bullet + 2\bullet \otimes \bullet + \bullet\,\bullet \otimes e, \\
\Delta(\overset{\bullet\,\bullet}{\underset{\bullet}{\vee}}) &= \overset{\bullet\,\bullet}{\underset{\bullet}{\vee}} \otimes e + (id_{\mathcal{H}} \otimes B^{+}) \circ \Delta(\bullet\,\bullet) \\
&= \overset{\bullet\,\bullet}{\underset{\bullet}{\vee}} \otimes e + (id_{\mathcal{H}} \otimes B^{+})(e \otimes \bullet\,\bullet + 2\bullet \otimes \bullet + \bullet\,\bullet \otimes e) \\
&= \overset{\bullet\,\bullet}{\underset{\bullet}{\vee}} \otimes e + \bullet\,\bullet \otimes \bullet + 2\bullet \otimes \overset{\bullet}{\underset{\bullet}{|}} + e \otimes \overset{\bullet\,\bullet}{\underset{\bullet}{\vee}}, \\
\Delta(3\bullet + 5\overset{\bullet}{\underset{\bullet}{|}}) = &= 3\,e \otimes \bullet + 3\bullet \otimes e + 5\,e \otimes \overset{\bullet}{\underset{\bullet}{|}} + 5\bullet \otimes \bullet + 5\overset{\bullet}{\underset{\bullet}{|}} \otimes e.
\end{aligned}
$$

A formula for the co-product

The co-product of a tree can also be computed by the formula (A. Connes & D. Kreimer 98) :

$$\Delta(t) \quad = \quad t \otimes e + e \otimes t + \sum_C P^C(t) \otimes R^C(t)$$

where C is the set of «admissibles» cut of the tree t, i.e. such that there is no more than one cut between any vertex of t and its root. A similar formula holds for forests (Murua 2003).

Elementary differentials

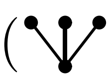
Definition 5 *For each* $t \in \mathcal{T}$*, the elementary differential* $F(t)$ *associated with* t *is the mapping from* $\mathbb{R}^n$ *to* $\mathbb{R}^n$*, defined recursively by :*

1. $F(\bullet)(y) = f(y)$,
2. $F([t_1, \ldots, t_n])(y) = f^{(n)}(y)\Big(F(t_1)(y), \ldots, F(t_n)(y)\Big)$.

Examples :

$F($  $)(y) \quad = \quad f'(y)f(y),$

$F($  $)(y) \quad = \quad f'(y)f'(y)f(y),$

$F($  $)(y) \quad = \quad f^{(3)}(y)\Big(f(y), f(y), f(y)\Big).$

B-series

Definition 6 (B-Series) *Let a be a mapping from $\mathcal{T}$ to $\mathbb{R}$. We define $B(a, y)$, the B-series associated with a, as the formal series :*

$$B(a, y) = y + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} a(t) F(t) = y + ha(\bullet) f(y) + h^2 a(\;)(f' f)(y) + \dots$$

The exact solution of $\dot{y} = f(y)$ has a B-series expansion

$$\begin{aligned} B(1/\gamma, y) &= y + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\gamma(t)\sigma(t)} F(t)(y) \\ &= y + hf(y) + \frac{h^2}{2.1}(f' f)(y) \\ &\quad + \frac{h^3}{3.2}(f''(f, f))(y) + \frac{h^3}{6.1}(f' f' f))(y) + \dots \end{aligned}$$

Most numerical methods have a formal B-series expansion

Examples :

1. Explicit Euler : $y + hf(y) = B(a, y)$ with $a(\bullet) = 1$ and $a(t \neq \bullet) = 0$.
2. Implicit Euler : $Y = y + hf(Y)$ and $y + hf(Y) = B(a, y)$ with $a(t) = 1$.

Classes of methods with a B-series expansion

1. Runge-Kutta methods
2. Composition methods
3. Multistep methods have an underlying B-series expansion

Classes of methods with a P-series expansion (decorated trees)

1. Splitting methods
2. Partitioned methods

Elementary differential operators

Definition 7 *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 :*

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

Examples :

$$\begin{aligned} X(e)[g] &= g, \\ X(\bullet)[g] &= g' f, \\ X\left(\begin{smallmatrix}\bullet\\ |\\ \bullet\end{smallmatrix}\right)[g] &= g' f' f, \\ X\left(\begin{smallmatrix}\bullet\\ |\\ \bullet\end{smallmatrix}\, \bullet\, \bullet\right)[g] &= g^{(3)}\Big(f' f, f, f\Big). \end{aligned}$$

S-series

Definition 8 (Series of differential operators) *Let α be a mapping from $\mathcal{F}$ into $\mathbb{R}$. We define $S(\alpha)$, the series of differential operators associated with α, as the formal series*

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

For all $g \in C^\infty(\mathbb{R}^n;\mathbb{R}^m)$:

$$S(\alpha)[g] = \alpha(e)g + h\alpha(\bullet)g'f + \frac{h^2}{2}\alpha(\bullet\,\bullet)g''(f,f) + h^2\alpha(\overset{\bullet}{\underset{\bullet}{|}})g'f'f + \ldots$$

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

Theorem 1 (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.*

$$B(a, B(b,y))$$

is again a B-series, with coefficients ab defined on $\mathcal{T}$ by the composition law :

$$\forall\, t\, \in \mathcal{T}, \quad (ab)(t) = (a \otimes b)\Delta(t).$$

Example :

$$\begin{aligned} (ab)(\vee) &= (a \otimes b)\Delta(\vee) \\ &= (a \otimes b)\Big(\vee \otimes e + (id_{\mathcal{H}} \otimes B^{+}) \circ \Delta(\bullet\,\bullet)\Big) \\ &= a(\vee)b(e) + a(\bullet)a(\bullet)b(\bullet) + 2a(\bullet)b(/) + a(e)b(\vee) \end{aligned}$$

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

Theorem 2 (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 the composition law :

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

Example :

$$\begin{aligned} (\alpha\beta)(\bullet\bullet\bullet) &= (\alpha \otimes \beta)\Delta(\bullet^3) \\ &= (\alpha \otimes \beta)\Big(\bullet \otimes e + e \otimes \bullet\Big)^3 \\ &= \alpha(\bullet^3)\beta(e) + 3\alpha(\bullet^2)\beta(\bullet) + 3\alpha(\bullet)\beta(\bullet^2) + \alpha(e)\beta(\bullet^3) \end{aligned}$$

Remarks and preliminary computations

– A B-series is a S-series :

$$B(a,y) = S(\alpha)[id_{\mathbb{R}^n}](y)$$

avec $\alpha_{|\mathcal{T}} \equiv a$.

– A S-series can be viewed as a Lie derivative operator (or a field) :

$$S(\alpha)[g](y) = L_{B(\alpha,y)}[g](y)$$

iff $\forall\, u \in \mathcal{F}/\mathcal{T},\ \alpha(u) = 0$.

– The action of a fonction g on a B-series can be viewed as S-series :

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

iff $\alpha \in Alg(\mathcal{H},\mathbb{R})$ et $\alpha_{|\mathcal{T}} \equiv a$.

Numerical methods preserving invariants

Let I be a first integral of $\dot{y} = f(y)$, i.e.

$$\forall\, y \,\in\, \mathbb{R}^n,\ \Big(\nabla I(y)\Big)^T f(y) = 0.$$

The numerical method associated with the B-series $B(a, y)$ preserves I iff

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

i.e.

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

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

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

In algebraic terms, saying that I is an invariant can be written

$$X(\,\bullet\,)[I] = 0.$$

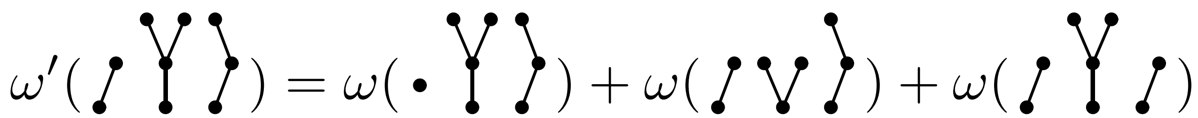
If $S(\omega)$ acts on $X(\,\bullet\,)[I]$ from the left, one gets :

$$S(\omega)[hX(\,\bullet\,)[I]] = S(\omega')[I] = 0,$$

with

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

<u>Example :</u>



The annihilating left ideal $\mathcal{I}[I]$ of I (part II)

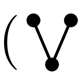
Lemma 1 *Consider $\delta \in \mathcal{H}^*$. Then, $\delta \in \mathcal{I}[I]$ if and only if $\delta(e) = 0$ and for all trees $t_1, \ldots, t_m$ de $\mathcal{T}$, one has :*

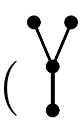
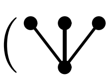
$$\delta(t_1 \ldots t_m) = \sum_{j=1}^{m} \delta\Big(t_j \circ \prod_{i \neq j} t_i\Big).$$

Notation :

$$s \circ (t_1 t_2 \ldots t_m) = B^+\Big(B^-(s) t_1 t_2 \ldots t_m\Big).$$

Examples :

– Pour $m = 2$: $\delta(\bullet$  $) = \delta($  $) + \delta($  $)$.

– Pour $m = 3$: $\delta($  $\bullet \bullet) = 2\delta($  $) + \delta($  $)$

Integrators preserving general invariants

Theorem 3 *Let $\alpha \in \mathrm{Alg}(\mathcal{H}, \mathbb{R})$. Then α satifies $S(\alpha)[I] = I$ 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 4 *A B-series integrator that preserves all cubic polynomial invariants does in fact preserve polynomial invariants of any degree, and thus is the B-series corresponding to the (scaled) exact flow.*

Consequence : There remains hope only for quadratic invariants.

Integrators preserving quadratic invariants

Theorem 5 *Let $\alpha \in \mathrm{Alg}(\mathcal{H}, \mathbb{R})$. Then α satifies $S(\alpha)[I] = I$ that for all couples (f, I) of a vector field f and a quadratic first integral I, if and only if $\alpha(e) = 1$ and α satisfies the condition*

$$\boxed{\alpha(t_1)\alpha(t_2) \quad = \quad \alpha(t_1 \circ t_2) + \alpha(t_2 \circ t_1)}$$

for all pairs $(t_1, t_2) \in \mathcal{T}^2$.

Example : A B-series integrator $B(a, y)$ preserve quadratic invariants ($m = 2$) if and only if, for all pairs of trees $(t_1, t_2) \in \mathcal{T}^2$, the following relation holds :

$$a(t_1 \circ t_2) + a(t_2 \circ t_1) = a(t_1)a(t_2).$$

This condition is also the condition for $B(a, y)$ to be symplectic.

Integrators preserving Hamiltonian invariants

We now turn our attention to systems of the form $\dot{y} = f(y)$ with

$$\boxed{f(y) \quad = \quad J^{-1}\nabla H(y),}$$

and we explore the conditions under which a B-series integrator $B(a, y)$ preserves exactly the Hamiltonian function, i.e.

$$S(\alpha)[H] = H$$

where α is the only algebra morphism such that $\alpha_{|\mathcal{T}} \equiv a$.

Elementary Hamiltonians

We define the *elementary Hamiltonian* $H(t)$ as the mapping from $\mathbb{R}^n$ to $\mathbb{R}$ obtained recursively by :

$$\begin{aligned}
H(\bullet)(y) &= H(y), \\
H([s_1, \ldots, s_n, t]) &= H^{(n+1)}\Big(F(s_1), \ldots, F(s_n), F(t)\Big), \\
&= \Big(F(t)\Big)^T J \left(J^{-1}\nabla H\right)^{(n)}\Big(F(s_1), \ldots, F(s_n)\Big) \\
&= \Big(F(t)\Big)^T JF(s) = H(s \circ t)
\end{aligned}$$

Lemma 2 *Let s and t be two trees of $\mathcal{T}$. We have the relation :*

$$H(s \circ t) = -H(t \circ s).$$

The annihilating ideal $\mathcal{I}[H]$ of H (part I)

Since $X(u)[H] = H(B^+(u)) = H([u])$, a lot of forests $u \in \mathcal{F}$ give rise to the same elementary differential.

Examples :

$$\begin{aligned} X(\;)[H] &= H(\;) = H(\bullet \circ \;) = -H(\; \circ \bullet) = -H(\;) \\ &= -X(\bullet\,\bullet)[H], \end{aligned}$$

$$X(\;\bullet)[H] = H(\;) = H(\; \circ \;) = 0$$

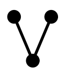
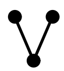
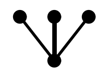
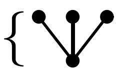
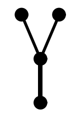
Auxiliary consequence :

One has $\frac{1}{h}B(b,y) = J^{-1}\nabla H_h(y)$ with $H_h(y) = S(\alpha)[H]$ iff

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

The set $\mathcal{HS}$ of non-superfluous free trees

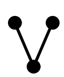
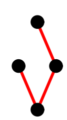
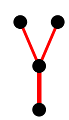
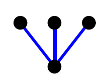
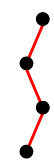
We define an equivalence class $\hat{t}$ as being the set of trees that can be obtained from t by changing the position of the root.

Examples : For $t =$ , $\hat{t} = \{$ ,  $\}$. For $t =$ , $\hat{t} = \{$ ,  $\}$.

Given a total order $\geq$ on $\mathcal{T}$, compatible with $|\cdot|$, the set $\mathcal{HS}$ is defined by

$$t \in \mathcal{HS} \text{ iff } t = \bullet \text{ or } \exists\,(s_1, s_2) \in \mathcal{T}^2,\ s_1 > s_2,\ \ t = s_1 \circ s_2.$$

The set $\mathcal{HS}$ is the set of representatives of equivalence classes whose elementary differential does not vanish. The first of these are :

 $\notin \mathcal{HS}$,  $\notin \mathcal{HS}$,  $\in \mathcal{HS}$,  $\notin \mathcal{HS}$,  $\notin \mathcal{HS}$,  $\in \mathcal{HS}$,  $\notin \mathcal{HS}$.

An algebraic condition for the preservation of Hamiltonians

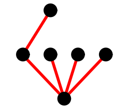
Writing the S-series in terms of elementary Hamiltonians :

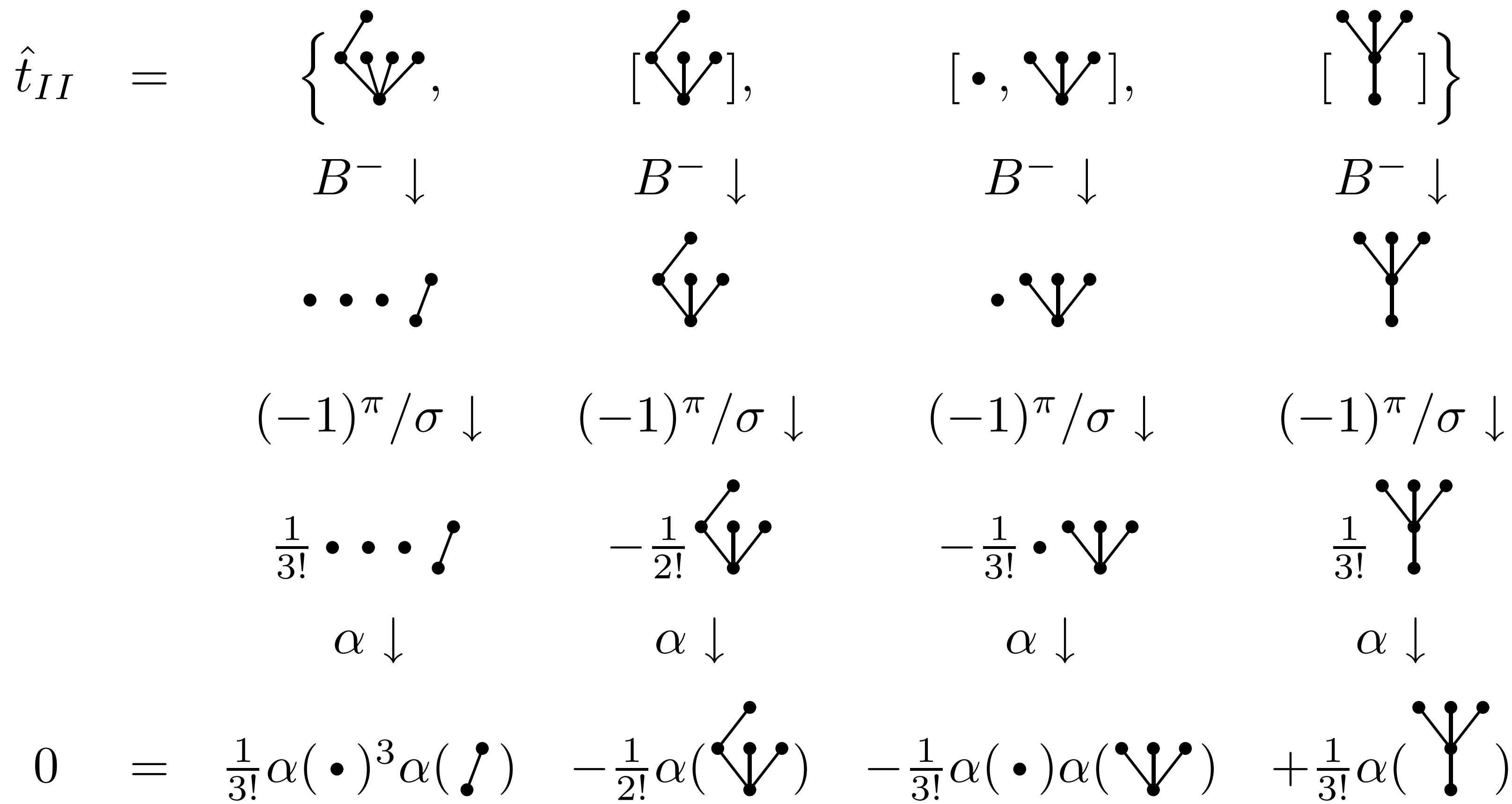
$$
\begin{aligned}
S(\alpha)[H] - H &= \sum_{u \in \mathcal{F}} \frac{h^{|u|}}{\sigma(u)} \alpha(u) X(u)[H] - H \\
&= \sum_{t \in \mathcal{HS} \backslash \{\bullet\}} h^{|t|-1} H(t) \sum_{u \in \mathcal{F},\, [u] \in \hat{t}} \frac{(-1)^{\pi([u])}}{\sigma(u)} \alpha(u).
\end{aligned}
$$

$\pi([u])$ is the «distance» between the root of $[u]$ and the root of t. Since the elementary Hamiltonians $H(t), t \in \mathcal{HS} \backslash \{\bullet\}$ are independent :

Theorem 6 *Let $\alpha \in \mathrm{Alg}(\mathcal{H}, \mathbb{R})$. One has $S(\alpha)[H] = H$ for all Hamiltonian systems, if and only if $\alpha(e) = 1$ and*

$$
\boxed{\forall\, t \in \mathcal{HS},\ \sum_{u \in \mathcal{F},\, [u] \in \hat{t}} (-1)^{\pi([u])} \frac{\alpha(u)}{\sigma(u)} = 0.}
$$

Example : the fifth-order condition for $t_{II} =$ 



The non-existence of symplectic Hamiltonian preserving integrators

Theorem 7 *Suppose a B-series integrator* $B(\alpha, y)$ *satisfies both conditions*

$$\forall\,(t_1, t_2)\,\in\,\mathcal{T}^2, \qquad \alpha(t_1)\alpha(t_2) = \alpha(t_1 \circ t_2) + \alpha(t_2 \circ t_1)$$

$$\forall\, t \in \mathcal{HS}, \qquad \sum_{u \in \mathcal{F},\ [u] \in \hat{t}} (-1)^{\pi([u])} \frac{\alpha(u)}{\sigma(u)} = 0.$$

for the preservation of quadratic invariants and for the preservation of exact Hamiltonians. Then it is the B-series of the scaled exact flow.

There exists no symplectic numerical method that preserves the Hamiltonian exactly

Symplectic methods are formally conjugate to a method that preserve the Hamiltonian exactly

Theorem 8 *Consider a symplectic integrator $B(\alpha, y)$. Then, there exists $\tilde{\gamma} \in \mathrm{Alg}(\mathcal{H}, \mathbb{R})$ such that the integrator associated with $\tilde{\alpha} = \tilde{\gamma}^{-1}\alpha\tilde{\gamma}$ exactly preserves the Hamiltonians.*

$$
\begin{array}{ccccccc}
\tilde{y}_0 & \xrightarrow{\tilde{\alpha}} & \tilde{y}_1 & \xrightarrow{\tilde{\alpha}} & \ldots & \xrightarrow{\tilde{\alpha}} & \tilde{y}_n \\
\downarrow \tilde{\gamma} & & \downarrow \tilde{\gamma} & & \downarrow \tilde{\gamma} & & \downarrow \tilde{\gamma} \\
y_0 & \xrightarrow{\alpha} & y_1 & \xrightarrow{\alpha} & \ldots & \xrightarrow{\alpha} & y_n
\end{array}
$$

PART II : modified equations

Backward error analysis

The fundamental idea of backward error analysis consists in interpreting the numerical solution $y_1 = \Phi_h^f(y_0)$

$$\begin{aligned} \dot{y} &= f(y), \\ y(0) &= y_0, \end{aligned}$$

as the exact solution of a modified differential equation

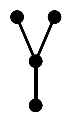
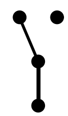
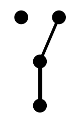
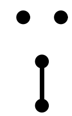
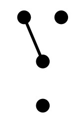
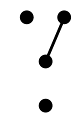
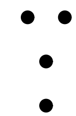
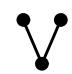
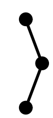
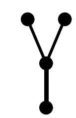
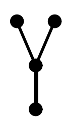
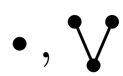
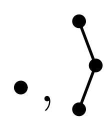
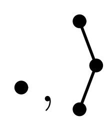
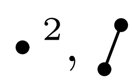
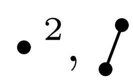
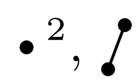
$$\begin{aligned} \dot{\hat{y}} &= \hat{f}(\hat{y}), \\ \hat{y}(0) &= y_0. \end{aligned}$$

Partitions and skeletons

Definition 9 ***(Partitions of a tree)*** *The partition p^τ of a tree $\tau \in \mathcal{T}$ is the tree obtained from τ by replacing some of its edges by dashed ones. We denote $P(p^\tau) = \{s_1, \ldots, s_k\}$ the list of subtrees $s_i \in \mathcal{T}$ obtained from p^τ by removing dashed edges. The set of all partitions p^τ of τ is denoted $\mathcal{P}(\tau)$.*

Definition 10 *The* skeleton $\chi(p^\tau) \in \mathcal{T}$ *of a partition $p^\tau \in \mathcal{P}(\tau)$ of a tree $\tau \in \mathcal{T}$ is the tree obtained by replacing in p^τ each tree of $P(p^\tau)$ by a single vertex and then dashed edges by solid ones. We can notice that $|\chi(p^\tau)| = \#p^\tau$.*

Example : The 8 partitions of tree $\tau = [[\bullet, \bullet]]$ with corresponding skeletons and lists

$p^\tau \in \mathcal{P}(\tau)$								
$\#p^\tau$	1	2	2	2	3	3	3	4
$\chi(p^\tau)$								
$P(p^\tau)$								

A substitution law

Theorem 9 *Let a, b be two mappings from $\mathcal{T} \cup \{e\}$ to $\mathbb{R}$ with $b(e) = 0$ and consider the (h-dependent) field*

$$hg_h(y) = B_f(b, y).$$

Then, there exists a mapping $a \star b$ from $\mathcal{T} \cup \{e\}$ to $\mathbb{R}$ satisfying

$$B_{g_h}(a, y) = B_f(a \star b, y).$$

and $a \star b$ is defined by $a \star b(e) = a(e)$ and for all τ in $\mathcal{T}$:

$$\boxed{a \star b(\tau) = \sum_{p^\tau \in \mathcal{P}(\tau)} a(\chi(p^\tau)) \prod_{\delta \in P(p^\tau)} b(\delta).}$$

A few terms of the substitution law

$$
\begin{aligned}
a \star b(\bullet) &= a(\bullet)b(\bullet),\\
a \star b([\bullet]) &= a(\bullet)b([\bullet]) + a([\bullet])b(\bullet)^2,\\
a \star b([\bullet\bullet]) &= a(\bullet)b([\bullet\bullet]) + 2a([\bullet])b(\bullet)b([\bullet]) + a([\bullet\bullet])b(\bullet)^3,\\
a \star b([[\bullet\bullet]]) &= a(\bullet)b([[\bullet\bullet]]) + a([\bullet])b(\bullet)b([\bullet\bullet]) + 2a([\bullet])b(\bullet)b([[\bullet]])\\
&\quad + a([\bullet\bullet])b(\bullet)^2 b([\bullet]) + 2a([[\bullet]])b(\bullet)^2 b([\bullet]) + a([[\bullet\bullet]])b(\bullet)^4,\\
a \star b([[[\bullet]]]) &= a(\bullet)b([[[\bullet]]]) + 2a([\bullet])b(\bullet)b([[\bullet]]) + a([\bullet])b([\bullet])^2\\
&\quad + 3a([[\bullet]])b(\bullet)^2 b([\bullet]) + a([[[\bullet]]])b(\bullet)^4.
\end{aligned}
$$

Main result

Theorem 10 *There exists a modified field* $\hat{f}_h(y) = \frac{1}{h}B(\hat{b}, y)$ *such that*

$$\Phi_h^f(y_0) = \hat{y}(h),$$

where $\hat{y}(t)$ *denotes the exact solution of*

$$\hat{y}(0) = y_0, \qquad \dot{\hat{y}} = \hat{f}_h(\hat{y}).$$

The coefficients $\hat{b}$ *are given by*

$$\hat{b} = \omega \star (a - \delta_e),$$

where $\frac{1}{h}B(\omega, y)$ *can be interpreted as the B-series expansion of the modified field for the Euler explicit method.*

Main consequence

Theorem 11 *Consider a B-series with coefficients a satisfying the condition :*

$$\forall m,\ 2 \leq m \leq n, \quad \forall (u_1, \ldots, u_m) \in \mathcal{T}^m, \quad \sum_{i=1}^{m} a(u_i \circ \prod_{j \neq i} u_j) = \prod_{i=1}^{m} a(u_i).$$

Then the coefficients $\hat{b}$ of its modified equation satisfy :

$$\forall m,\ 2 \leq m \leq n, \quad \forall (u_1, \ldots, u_m) \in \mathcal{T}^m, \quad \sum_{i=1}^{m} b(u_i \circ \prod_{j \neq i} u_j) = 0.$$

The converse is also true.