Rooted trees

Definition

Let T be the set of non-planar trees defined as follows. A non-planar Butcher tree is a rooted tree defined recursively by

$$\bullet \in T, \quad (\tau_n, \ldots, \tau_1)_\bullet \in T, \quad \tau_1, \ldots, \tau_n \in T,$$

where the root is graphically represented at the bottom. $(\tau_n, \ldots, \tau_1)_\bullet$ denotes the tree with the root $\bullet$ and the n trees $\tau_n, \ldots, \tau_1$ plugged to the root.

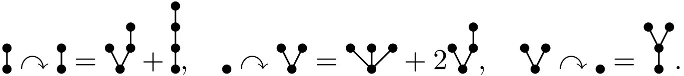
Remark

By non-planar, we mean that the order of the branches does not matter: for instance,  $=$ .

Grafting

The grafting of trees $\curvearrowright$ is defined as a product on T returning the sum of all possibilities (counted with multiplicity) of grafting the root of one tree on the nodes of another tree.

Example



By extending $\curvearrowright$ linearly on $\mathcal{T} = \mathsf{Span}_{\mathbb{R}}(T)$, this defines the pre-Lie algebra $(\mathcal{T}, \curvearrowright)$ of Butcher trees.

Remark

A natural grading on $\mathcal{T}$ is given by the number of nodes: $|$$| = 3$.

$$\forall \tau_1, \tau_2 \in T, \quad |\tau_1 \curvearrowright \tau_2| = |\tau_1| + |\tau_2|.$$

The elementary differential map

$$\left.\begin{array}{ll} \mathfrak{p} & : \mathbb{G} \twoheadrightarrow M \text{ the cotangent projection} \\ 0 & : M \to \mathbb{G} \text{ the zero section of } \mathbb{G} \end{array}\right. . \text{ Let } H \in \mathcal{C}^\infty(M).$$

Definition (Elementary differential map)

The elementary differential map $\mathbb{F}^H \colon \mathcal{T} \to \mathcal{C}^\infty(M)$ associated to H is defined by

$$\mathbb{F}^H(\bullet) = H \quad \text{and}$$

$$\mathbb{F}^H\Big((\tau_n, \ldots, \tau_1)_\bullet\Big) = 0^*\{\{\ldots\{\alpha^* H, \mathfrak{p}^*\mathbb{F}^H\big(\tau_1\big)\}_\omega, \ldots\}_\omega, \mathfrak{p}^*\mathbb{F}^H\big(\tau_n\big)\}_\omega.$$

Example

$$\mathbb{F}^H\Big(\begin{smallmatrix}\bullet\\ |\\ \bullet\end{smallmatrix}\Big) = 0^*\{\alpha^* H, \mathfrak{p}^* H\}_\omega.$$

Idea

Compute the terms of the Taylor series of the Hamilton-Jacobi equation by grafting trees and apply $\mathbb{F}^H$.

Butcher series

Definition (Butcher series)

The B-series associated to $H \in \mathcal{C}^\infty(M)$ is the following formal series indexed by a coefficient map $a \in \mathcal{T}^*$:

$$B^H : \begin{array}{ccc} \mathcal{T}^* & \to & \mathcal{C}^\infty(M)\left[[t]\right] \\ a & \mapsto & \sum_{\tau \in T} \frac{a(\tau)}{\sigma(\tau)} \mathbb{F}^{tH}(\tau) \end{array}$$

where $\sigma(\tau)$ is the number of graph automorphisms of τ, also called the symmetry coefficient.[2]

Remark

For any $\tau \in \mathcal{T}, \mathbb{F}^{tH}(\tau) \in \mathcal{C}^\infty(M)\left[t\right]$. *Actually,* $deg(\mathbb{F}^{tH}(\tau)) = |\tau|$.

[2] See Geometric Numerical Integration, Hairer et al., 2006, sec. III.1, for an explicit formula of the symmetry coefficient.

Formal solution of HJ equation

Lemma

For any $(S_t)_{t\in I} \in \mathcal{C}^\infty(M \times I)$ *and any* $(f_t)_{t\in I} \in \mathcal{C}^\infty(T^*M \times I)$,

$$\frac{\partial}{\partial t}\left((dS_t)^* f_t\right) = (dS_t)^* \left(\{f_t, \mathfrak{p}^* \frac{\partial S_t}{\partial t}\}_\omega + \frac{\partial f_t}{\partial t}\right). \tag{4}$$

Theorem (Busnot Laurent, O.C., 2025)

Let $(S_t)_{t\in I} \in \mathcal{C}^\infty(M \times I)$ *be the solution of the Hamilton-Jacobi equation* (2)*, then its Taylor expansion is given by*

$$B^H(e) \in \mathcal{C}^\infty(M)[[t]], \tag{5}$$

where $e \in \mathcal{T}^*$ *is given by*

$$e(\bullet) = 1, \quad e(\tau) = \frac{1}{|\tau|} e(\tau_1) \dots e(\tau_n), \quad \tau = (\tau_n, \dots, \tau_1)_\bullet.$$

Explicit construction through birealisations

Let π a Poisson structure on $\mathbb{R}^d$. Assume that a birealisation (α, β) is constructed for π. Let $H \in \mathcal{C}^\infty(\mathbb{R}^n)$, $k \in \mathbb{N}$ and $\Delta t > 0$ a time-step.

1. Solve the Hamilton-Jacobi equation up to order k using Butcher series of Equation (5). Obtain $S^k_{\Delta t} \in \mathcal{C}^\infty(M)$.
2. Let $x_n \in \mathbb{R}^d$. Solve the nonlinear equation

   $$\alpha(\bar{x}_n, \nabla_{\bar{x}_n} S^k_{\Delta t}) = x_n$$

   by a fixed point method, e.g., Newton descent.
3. One step of the obtained Hamiltonian Poisson integrator of order k and time-step Δt is then given by

   $$x_{n+1} = \beta(\bar{x}_n, \nabla_{\bar{x}_n} S^k_{\Delta t}).$$

Expected numerical behaviour

- **stay on a leaf** because the numerical methods are induced by bisections
- **stability near a singularity** because these bisections are Lagrangian
- **oscillate around first integrals** as symplectic numerical methods do

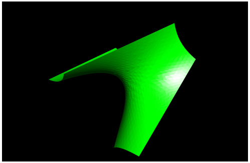
Poisson structure and foliation of a cluster Poisson structure on $\mathbb{R}^3$

- **the Poisson bracket**

$$\{f,g\}(x) = (\nabla_x f)^T \cdot \begin{pmatrix} 0 & x_1x_2 & x_1x_3 \\ -x_1x_2 & 0 & x_2x_3 \\ -x_1x_3 & -x_2x_3 & 0 \end{pmatrix} \cdot \nabla_x g$$

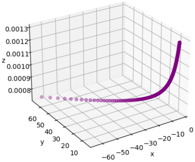
- **a bi-realisation** $\begin{cases} \alpha\colon (x,p) \mapsto \begin{pmatrix} e^{\frac{1}{2}(x_2p_2+x_3p_3)}x_1 \\ e^{\frac{1}{2}(-x_1p_1+x_3p_3)}x_2 \\ e^{-\frac{1}{2}(x_1p_1+x_2p_2)}x_3 \end{pmatrix} \\ \beta\colon (x,p) \mapsto \alpha(x,-p) \end{cases}$,

- **a symplectic leaf**



A Hamiltonian vector field with an exploding trajectory

$$H(x) = \sum_{i=1}^{3} x_i \Rightarrow \begin{cases} \dot{x_1} = & x_1(x_2 + x_3) \\ \dot{x_2} = & x_2(-x_1 + x_3) \\ \dot{x_3} = & -x_3(x_1 + x_2) \end{cases}$$

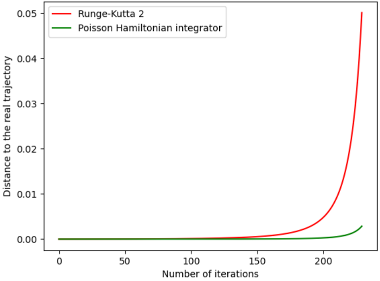


$$\begin{cases} \lim\limits_{t\to\infty} x_1(t) = & -\infty \\ \lim\limits_{t\to\infty} x_2(t) = & \infty \\ \lim\limits_{t\to\infty} x_3(t) = & 0 \end{cases}.$$

Exploding for $\begin{pmatrix} x_1(0) \\ x_2(0) \\ x_3(0) \end{pmatrix} = \begin{pmatrix} -3 \\ 5 \\ 10^{-3} \end{pmatrix}$

(Vanhaecke et al. 2016)

Numerical simulation: comparison of numerical errors



Error with respect to the analytical solution

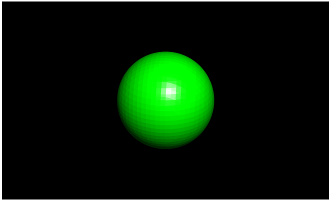
with initial point $\begin{pmatrix} -3 \\ 5 \\ 10^{-3} \end{pmatrix}$ and $\Delta t = 10^{-3}$.

Poisson structure and foliation of $so(3)^*$

- **the Poisson bracket**

$$\{f, g\}(x) = (\nabla_x f)^T \cdot \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix} \cdot \nabla_x g$$

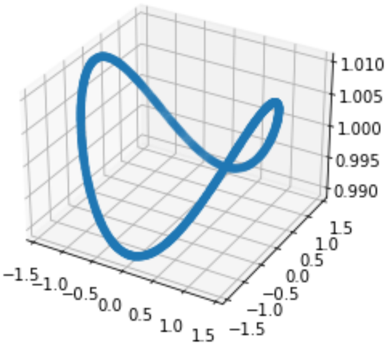
- **a bi-realisation** $\mathbb{R}^3 \simeq so(3)$ $\begin{cases} \alpha\colon (x, p) \mapsto (I + \frac{p}{2}).x.(I - \frac{p}{2}) \\ \beta\colon (x, p) \mapsto \alpha(x, -p) \end{cases}$
- **a symplectic leaf**



The Hamiltonian vector field of angular velocity of a rigid body in $\mathbb{R}^3$

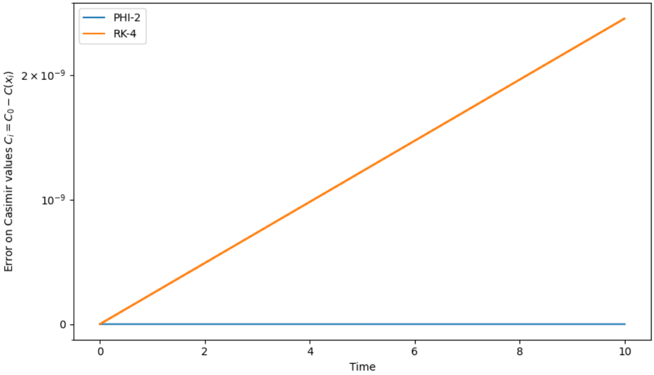
$$H(x) = \frac{1}{2}\Big(i_1(x_2^2 + x_3^2) + i_2(x_1^2 + x_3^2) + i_3(x_1^2 + x_2^2)\Big)$$

$$\Rightarrow \dot{x} = -x \wedge I.x$$



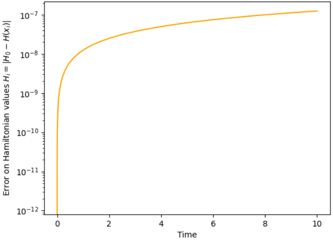
$x(0) = (1, 1, 0)$

Preservation of Casimir levels

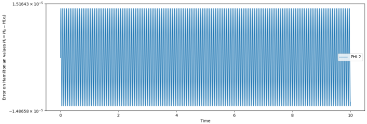


Error on Casimir values for HPI-2 and RK-4

Controlled oscillations around Hamiltonian levels



Errors on Hamiltonian values for RK-4



Errors on Hamiltonian values for HPI-2

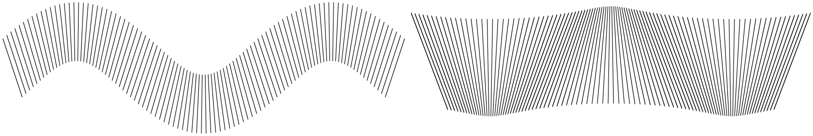
Exercises

1. Use the lemma of Equation (4) to compute the terms of order 1 and 2 of the solution of the Hamilton-Jacobi equation (2).
2. Verify that the Butcher series of the equation (5) solves the Hamilton-Jacobi equation at order 2.

Bibliography for the third lecture

- *Numerical Methods in Poisson Geometry and Applications to Mechanics*, O. C., C. Laurent-Gengoux, V. Salnikov, Mathematics and Mechanics of Solids, 2024
- *Butcher series for Hamiltonian Poisson integrators through symplectic groupoids*, A. Busnot Laurent, O. C., arXiv, 2025

Poisson integrators for the Timoshenko model (w. L. Le Marrec, V. Carlier)



Two beam configurations

fig: Le Marrec

Hamiltonian structure of Timoshenko model[3]

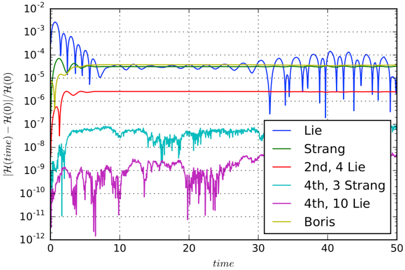
- compute a birealisation
- construct Hamiltonian Poisson integrators
- expect these numerical methods to track periodic orbits efficiently, detect instabilities...

[3] *Timoshenko beam under finite and dynamic transformations: Lagrangian coordinates and Hamiltonian structures*, O.C. & Le Marrec, 2025

Construction of birealisations by perturbative techniques

- Construct birealisations by studying deformation theory of symplectic groupoids
  $\rightarrow$ several ongoing discussions with D. Calaque, A. Busnot Laurent, V. Dotsenko

- Poisson integrators in plasma physics with É. Sonnendrucker



Landau damping: energy error[4]

[4] GEMPIC, Sonnendrucker et al., 2017