# Invariant theory of Hamiltonian mechanics and related numerical analysis

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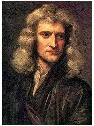
# Geometric mechanics



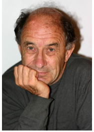
Isaac **Newton**, 1643-1727

Émilie **du Châtelet**, 1706-1749

Joseph-Louis **de Lagrange**, 1736-1813

Siméon Denis **Poisson**, 1781-1840

Marius Sophus **Lie**, 1842-1899



Vladimir I. **Arnol'd**, 1937-2010

André **Lichnerowicz**, 1915-1998

and Carl Gustav Jacob **Jacobi** (1804 - 1851), Sir William Rowan **Hamilton** (1805 –1865), Sofia Vassilievna **Kovalevskaïa** (1850-1891), Henri **Poincaré** (1854-1912), Jean-Marie **Souriau** (1922 - 2012), Alan David **Weinstein** (1943- )...

# Definition

$M$ be a smooth manifold.
Recall that a Lie bracket on $\mathcal{C}^\infty(M)$ is a bilinear anti-symmetric map from $\mathcal{C}^\infty(M) \times \mathcal{C}^\infty(M) \to \mathcal{C}^\infty(M)$ such that

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0 \qquad \textit{(Jacobi relation)}.$$

## Definition (Flato, Lichnerowicz, Sternheimer, 1975)

A Poisson bracket on $M$ is a Lie bracket on $\mathcal{C}^\infty(M)$ such that for all $f, g, h \in \mathcal{C}^\infty(M)$,

$$\{fg, h\} = f\{g, h\} + \{f, g\}h \qquad \textit{(Leibniz rule)}.$$

**Remark**

*Anti-symmetry of* $\{.,.\} \Rightarrow$ *for all* $H \in \mathcal{C}^\infty(M)$, $\{H, H\} = 0$.

# Consequence of the Leibniz rule: Poisson tensor of $\{.,.\}$

## Lemma

*An $\mathbb{R}$-bilinear map $B\colon \mathcal{C}^\infty(M) \times \mathcal{C}^\infty(M) \to \mathcal{C}^\infty(M)$ arises from a smooth bivector field $\pi \in \Gamma(\bigwedge^2 TM)$ by the formula*

$$B(f,g) = \langle \pi, df \wedge dg \rangle$$

*if and only if $B$ is skew-symmetric and verifies the Leibniz rule*

$$B(fg,h) = fB(g,h) + B(f,g)h$$

### Corollary

*Any Poisson bracket $\{\cdot,\cdot\}$ gives rise to a smooth bivector field $\pi \in \Gamma(\bigwedge^2 TM)$ . If $(x_i)_i$ are coordinates on $M$, $\pi_{i,j} = \{x_i, x_j\}$.*

**Remark**

*This holds because we assumed $M$ to be finite dimensional.*

# Two consequences of the Jacobi relation

### Proposition (Poisson brackets are particular cases of bivector fields)

*There is a $1$-to-$1$ correspondence between Poisson brackets on $M$ and smooth bivector fields $\pi$ such that the map*

$$(f, g) \in \mathcal{C}^\infty(M)^2 \mapsto \langle \pi, df \wedge dg \rangle$$

*satisfies the Jacobi relation.*

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### Definition

Let $H \in \mathcal{C}^\infty(M)$. $f \in \mathcal{C}^\infty(M)$ is a first integral of $H$ if $\{H, f\} = 0$.

### Proposition (Poisson theorem)

$\{H, f\} = \{H, g\} = 0 \Rightarrow \{H, \{f, g\}\} = 0.$

Jacobi cyclic relation implies a Lie algebra structure on the first integrals of $H$.

# A first example: symplectic manifolds

Let $M$ be a symplectic manifold, meaning a manifold equipped with a closed $2$-form $\omega$ such that for all $x \in M$, the map:

$$\omega^\flat \colon X \in T_xM \mapsto \omega_x(X, \cdot) \in T_x^*M$$

is a bijection, with inverse denoted by $\omega^\sharp$. The Poisson bracket of a symplectic manifold is

$$\{f, g\} = \langle \mathrm{d}f, \omega^\sharp(\mathrm{d}g) \rangle.$$

**Remark**

*Jacobi relation for this Poisson bracket is equivalent to the closedness of $\omega$.*

In Darboux coordinates $(q, p)$, the Poisson tensor is given by the matrix $\begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$ and the corresponding Poisson bracket

$$\{f, g\}(q, p) = \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial g}{\partial q}\frac{\partial f}{\partial p}.$$

# Two more examples

2nd example: Lie-Poisson structure on $\mathfrak{g}^*$

Let $\mathfrak{g}$ be a Lie algebra. $M = \mathfrak{g}^*$ comes canonically equipped with the Poisson bracket

$$\forall f, g \in \mathfrak{g}^*, \quad \forall x \in \mathfrak{g}, \quad \{f, g\}(x) = \langle x, [\mathrm{d}_x f, \mathrm{d}_x g] \rangle$$

where $\mathrm{d}_x f \in \mathfrak{g}^{**} \simeq \mathfrak{g}$.

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3rd example: Cluster Poisson brackets

Let $A = (a_{i,j})_{1 \leq i,j \leq n} \in \mathcal{M}_{n \times n}(\mathbb{R})$ anti-symmetric. Set $M = \mathbb{R}^n$ and

$$\forall x \in \mathbb{R}^n, \quad \forall 1 \leq i, j \leq n, \quad (\pi(x))_{ij} = a_{ij} x_i x_j.$$

# Poisson morphisms

## Definition

Let $(M_1, \{\cdot,\cdot\}_1)$ and $(M_2, \{\cdot,\cdot\}_2)$ two Poisson manifolds. A smooth map $\alpha\colon M_1 \to M_2$ is said to be a Poisson map, resp. an anti-Poisson map, if

$$\forall f, g \in \mathcal{C}^\infty(M_2), \qquad \{\alpha^* f, \alpha^* g\}_1 = \alpha^*\{f, g\}_2$$

$$\text{resp. } \{\alpha^* f, \alpha^* g\}_1 = -\alpha^*\{f, g\}_2.$$

## Example (Symplectic case)

Poisson automorphisms of a symplectic Poisson structure are called symplectomorphisms.

## Example (Linear case)

Linear Poisson automorphisms of the dual of a Lie algebra are transpose maps of automorphisms of the Lie algebra.

# Hamiltonian vector fields and flows

### Definition (Hamiltonian vector field)

Identifying $\mathfrak{X}(M) \simeq \mathrm{Der}(M)$, the Hamiltonian vector field of $H$ is set to be

$$X_H \colon \begin{array}{ccc} \mathcal{C}^\infty(M) & \to & \mathcal{C}^\infty(M) \\ f & \mapsto & \pi(\mathrm{d}H \wedge \mathrm{d}f) \end{array} .$$

### **Remark** (Hamiltonian systems are local)

*$X_H$ at $x \in M$ only depend on the differential $d_x H$ of $H$ at $x$.*

### Theorem

*The Hamiltonian flow $\phi_t^H$ of $H$ is a Poisson automorphism:*

$$\forall f, g \in \mathcal{C}^\infty(M), \quad \forall t, \quad (\phi_t^H)^*\{f, g\} = \{(\phi_t^H)^* f, (\phi_t^H)^* g\}$$

### Terminology

*Hamiltonian flows are said to be inner automorphisms of $\pi$.*

# 1st example of a Hamiltonian system: classical mechanics on $M = T^*X$

$$\begin{array}{ccc} X & \text{a smooth manifold} & \text{(the configuration space)} \\ \|\cdot\| & \text{a Riemannian metric on } X & \text{(the kinetic energy)} \\ V & \in \mathcal{C}^\infty(X) & \text{(the potential energy).} \end{array}$$

$$H\colon \begin{array}{ccc} T^*X & \to & \mathbb{R} \\ \zeta & \mapsto & \frac{1}{2m}\|\zeta\|^2 + V\circ\mathfrak{p}(\zeta) \end{array}$$

where: $\begin{array}{ll} \mathfrak{p}\colon T^*X \twoheadrightarrow V & \text{the cotangent projection} \\ m > 0 & \text{the mass.} \end{array}$

**Remark**

*The first integrals of $H$ depend on the physics. For instance: angular momentum.*

In cotangent coordinates $(q, p)$, the ODE of $X_H$ is:

$$\begin{cases} \dot{q} &= -\frac{p}{m} \\ \dot{p} &= \nabla V(q) \end{cases} \quad \text{i.e. 2nd law of Newton (1687) } m\ddot{q} = \nabla V(q)$$

# 2nd example of a Hamiltonian system: mechanics on $\mathfrak{g}^*$ and the angular velocity of a rigid body

For the **canonical Poisson structure on** $\mathfrak{g}^*$, the Hamiltonian system associated to $H \in \mathcal{C}^\infty(\mathfrak{g}^*)$ is

$$\dot{x} = \mathrm{ad}^*_{\mathrm{d}H} x$$

In the case of $so(3) \simeq \mathbb{R}^3$, the Poisson bracket is

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

The Hamiltonian of the angular velocity of the rigid body is

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

$$\Rightarrow \dot{x} = -x \wedge I.x, \text{ where } I = \begin{pmatrix} i_1 & 0 & 0 \\ 0 & i_2 & 0 \\ 0 & 0 & i_3 \end{pmatrix} \text{ is the inertia tensor}$$

# 3rd example of a Hamiltonian system: Lotka-Volterra system on a cluster Poisson structure

**the cluster Poisson bracket**

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

For the Hamiltonian

$$H(x) = \sum_{i=1}^{3} x_i$$

being the sum of the species populations, the corresponding Hamiltonian system is

$$\Rightarrow \begin{cases} \dot{x_1} = & x_1(x_2 + x_3) \\ \dot{x_2} = & x_2(-x_1 + x_3) \\ \dot{x_3} = & -x_3(x_1 + x_2) \end{cases} \tag{1}$$

**Remark** (Vanhaecke et al., 2016)

*The equation* (1) *has been proven to be part of a family of completely integrable systems.*

# First integrals

**Theorem**

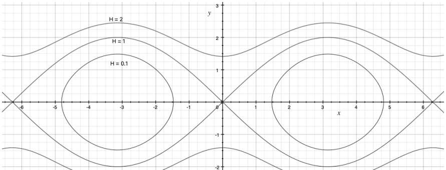
*Let $F \in \mathcal{C}^\infty(M)$ a first integral of $H$. The flow of $H$ commutes with the one of $F$:*

$$\forall s, t, \quad \phi_s^F \phi_t^H = \phi_t^H \phi_s^F$$

**Corollary**

*The Hamiltonian is always a preserved quantity along a trajectory of its Hamiltonian flow.*

In $\mathbb{R}^2$ equipped with $\pi = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, the data of the Hamiltonian levels of $H$ is enough to compute any integral curve of the Hamiltonian vector field of $H$.




Hyperbolic pendulum
$H(q, p) = \frac{p^2}{2} + \cos q$

# Casimir functions

### Definition

$C \in \mathcal{C}^\infty(M)$ is said to be a Casimir if it is a first integral for all smooth functions on $M$. Equivalently, its Hamiltonian vector field vanishes.

### Example (The non-degenerate case)

A symplectic Poisson structure has no non-trivial Casimir.

### Example (The linear case)

Any element of the center of a Lie algebra $\mathfrak{g}$ provides a Casimir on $\mathfrak{g}^*$.

### Example (A quadratic case)

Let $A$ be a $n \times n$ real anti-symmetric matrix and $(a_i)_{1 \leq i \leq n} \in \ker A$. Then, the function $x \in \mathbb{R}^n \mapsto \Pi_{i=1}^n x_i^{a_i}$ is a Casimir of the cluster Poisson bracket associated to the matrix $A$.

# Symplectic foliation

On a Poisson manifold $M$, not all the points can be connected by Hamiltonian flows. This foliates $M$.

**Theorem**

*Any Poisson manifold $(M, \pi)$ is foliated into symplectic leaves. This foliation is singular.*

A foliation is in particular a partition of the manifold into immersed submanifolds.
Let $x \in M$ and $\mathcal{F}_x$ the leaf of $x$.

- $\mathcal{F}_x$ is a symplectic manifold.
- The immersion $\mathcal{F}_x \hookrightarrow M$ is a Poisson morphism.
- Let $y \in M$. The topology of $\mathcal{F}_y$ might differ a lot from the one of $\mathcal{F}_x$, even if $x$ and $y$ are close.

**Remark**

*Any Casimir must be constant on a symplectic leaf.*

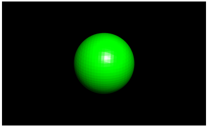
# Symplectic foliation of the examples

The symplectic Poisson structure

The symplectic foliation is made of one symplectic leaf: the whole space.

Lie-Poisson structure on $\mathfrak{g}^*$

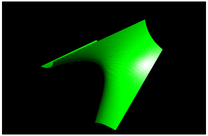
It is given by coadjoint orbits.



A symplectic leaf of $so(3)^* \simeq \mathbb{R}^3$

Cluster Poisson brackets

Exercise !



A symplectic leaf of $\{x_i, x_j\} = x_i x_j$,

# Properties of Hamiltonian flows

Let $H \in \mathcal{C}^\infty(M)$. Its Hamiltonian flow $\phi_t^H$

- **preserves** $H$**:** $H \circ \phi_t^H = H$,
  Hamiltonian flows are *conservative*.
- **preserves the Poisson tensor:** ${\phi_t^H}_\star \pi = \pi$,
  Hamiltonian flows are *inner automorphisms of the Poisson structure*.
- **stay on a leaf:** $\forall x \in M, \quad \phi_t^H(x) \in \mathcal{F}_x$,
  this provides a *construction* of any symplectic leaf, cf control theory.

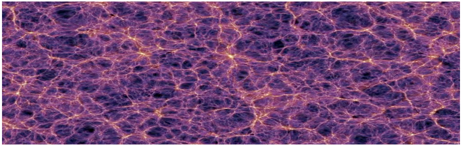
# Symplectic Runge-Kutta

Define an integrator as a family: $\varphi_\epsilon \colon x_n \mapsto x_{n+1}$ depending on the time-step $\epsilon$.

## Definition

In the space $\{(q,p)\}$ of position-momenta, an integrator $\varphi_\epsilon$ is said to be **symplectic** if it is a Poisson morphism for the Poisson structure $\pi(q,p) = \begin{pmatrix} 0 & -Id \\ Id & 0 \end{pmatrix} := J$.

Symplectic integrators are used in astrophysics, molecular dynamics, optics...



Virgo project, 2004

# How to cook up a symplectic integrator ?

Here: $\pi = J$.

A Runge-Kutta integrator for $\dot{x} = J \cdot \nabla_x H$ is of the form

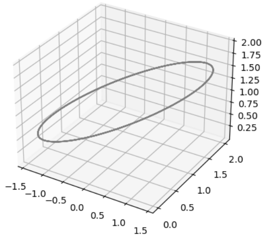
$$\begin{aligned} x_{n+1} &= x_n + \epsilon \sum_{i=1}^{s} b_i k_i \\ k_i &= J \cdot \nabla H(x_n + \epsilon \sum_{j=1}^{s} a_{ij} k_j) \end{aligned}$$

where $x := (q, p)$.

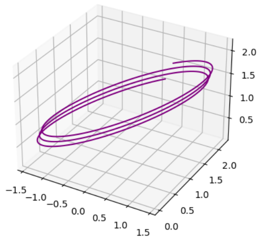
## Theorem

*If : $\forall (i,j)$, $b_i a_{ij} + b_j a_{ji} = b_i b_j$,*
*then the integrator is symplectic.*

# Runge-Kutta Poisson ?




A Hamiltonian trajectory for a Poisson structure in $\mathbb{R}^3$




An integrator that preserves this Poisson structure

In the general case, it is not enough to preserve the Poisson structure. Such an integrator, even of high order, may provide bad numerical simulations: *it destroys the foliation.*

# Exercises for next week

1. Prove that the cluster Poisson brackets are indeed Poisson brackets, namely, that the brackets verify the Jacobi relation.

2. Compute the symplectic foliation of $\mathbb{R}^3$ endowed with $\{x_1, x_2\} = x_1 x_2$, $\{x_1, x_3\} = 2x_1 x_3$, $\{x_2, x_3\} = x_2 x_3$. Namely: describe the partition of $\mathbb{R}^3$ induced by these Poisson brackets.

# Bibliography for the first lecture


- *Symplectic Geometry and Analytical Mechanics*, Paulette Libermann and Charles-Michel Marke, Kluwer, 1987
  → Poisson geometry and mechanics

- Chapter 1 of *Poisson Structures and their Normal Forms*, Jean-Paul Dufour and Nguyen Tien Zung, Birkhäuser, 2005
  → Basics on Poisson geometry

- *Lectures on Poisson Geometry*, Marius Crainic, Rui Loja Fernandes, Ioan Mărcuț, American Mathematical Society, 2021
  → More involved Poisson geometry