A Potpourri of Geometric Structures for Fluids and Plasmas

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Contact Geometry, General Relativity, and Thermodynamics

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Overview

I. Symplectic maps

- Magnetic devices and zonal flows

II. Flows on finite-dimensional Poisson manifolds

- Symplectic and Clebsch-Poisson integrators – the Kida vortex.

III. Metriplectic Dynamics (thermodynamically consistent systems)

IV. Comparison of Metriplectic Dynamics to Contact Hamiltonian Dynamics

V. Final Comments

I. Symplectic Maps

Hamilton's Canonical Equations

Phase Space with Canonical Coordinates: (q, p)

Hamiltonian function: $H(q, p)$ $\leftarrow$ the energy

Equations of Motion:

$$\boxed{\dot{p}_\alpha = -\frac{\partial H}{\partial q^\alpha}\,, \qquad \dot{q}^\alpha = \frac{\partial H}{\partial p_\alpha}\,,} \qquad \alpha = 1, 2, \ldots N$$

Phase Space Coordinate Rewrite: $z = (q, p)\,, \quad i, j = 1, 2, \ldots 2N$

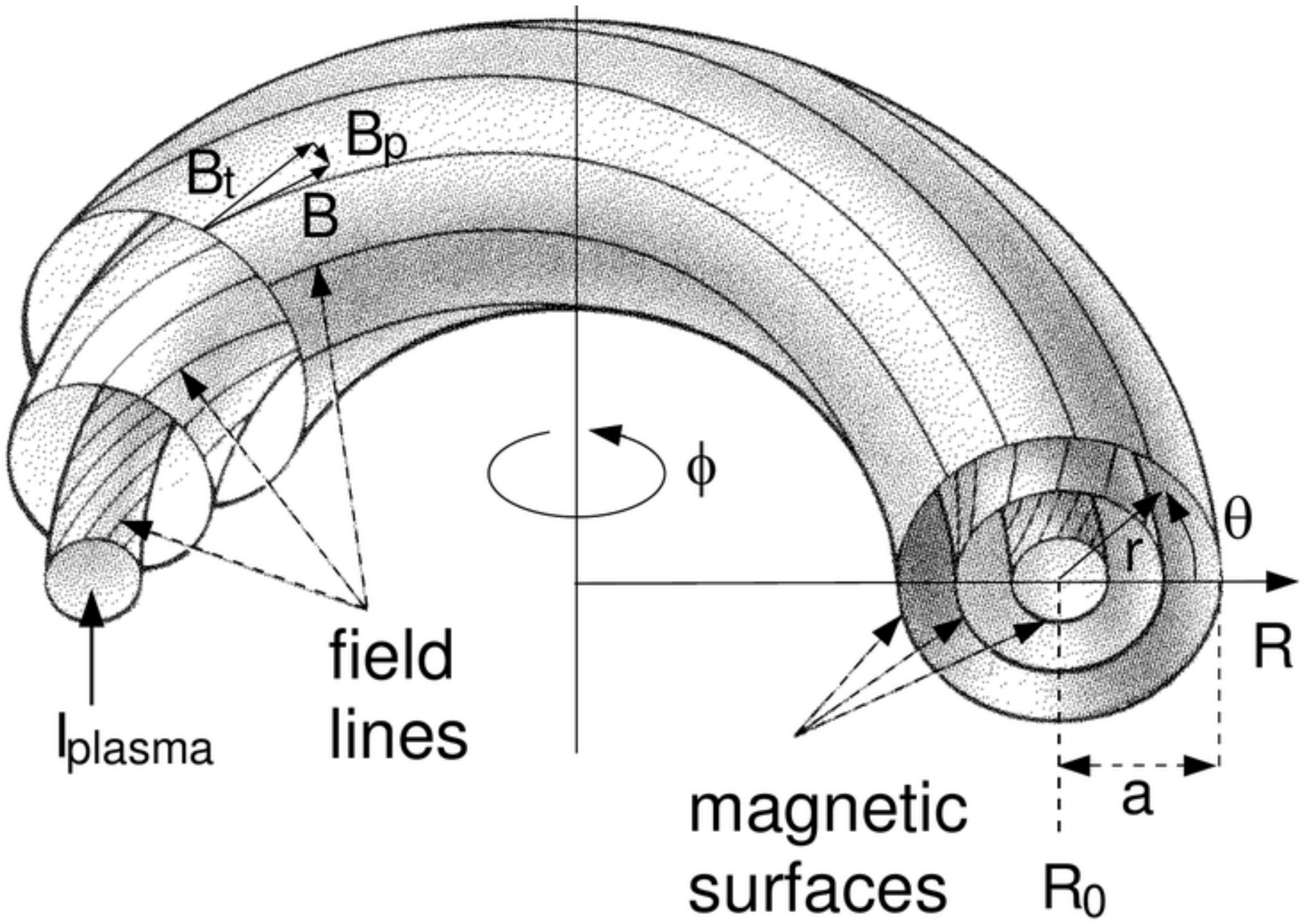
$$\dot{z}^i = J_c^{ij} \frac{\partial H}{\partial z^j} = \{z^i, H\}_c\,, \qquad (J_c^{ij}) = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix},$$

$J_c :=$ Poisson tensor, Hamiltonian bi-vector, cosymplectic form

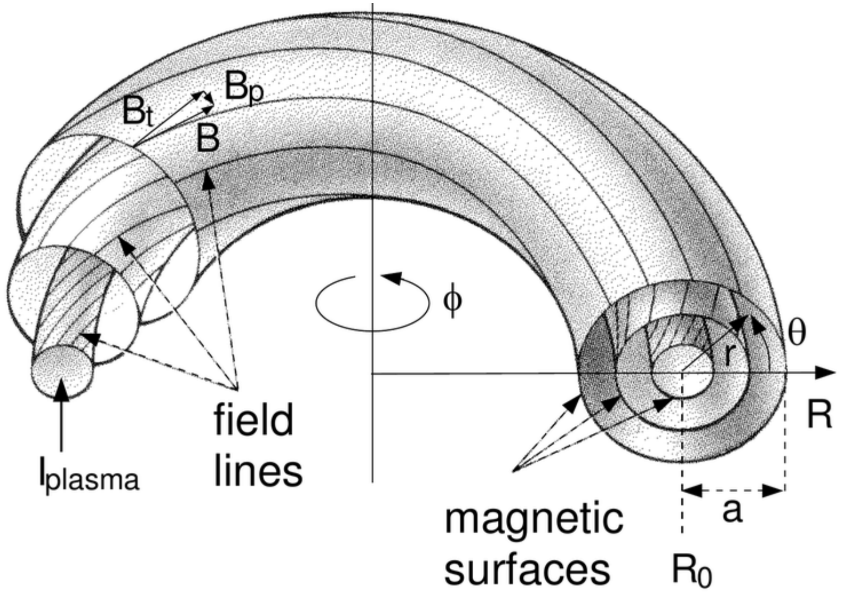
Two Physical Systems

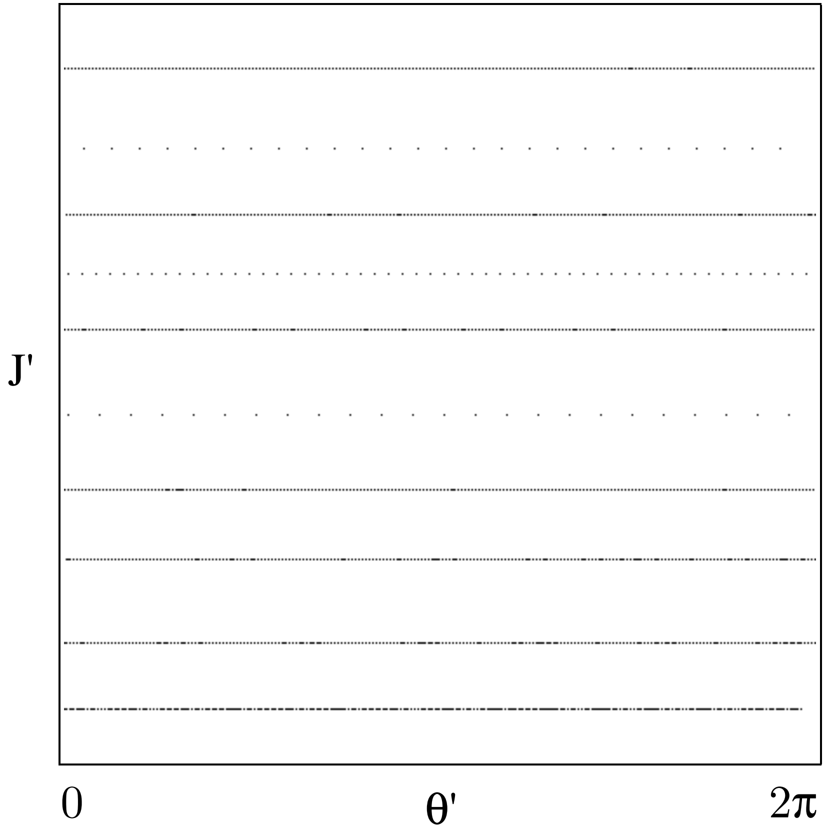
- Magnetic plasma confinement devices $\longleftarrow$
- Zonal flows of atmospheric polar vortex an anular flow

Magnetic field lines as symplectic map (Kruskal 1952) in toroidal plasma device

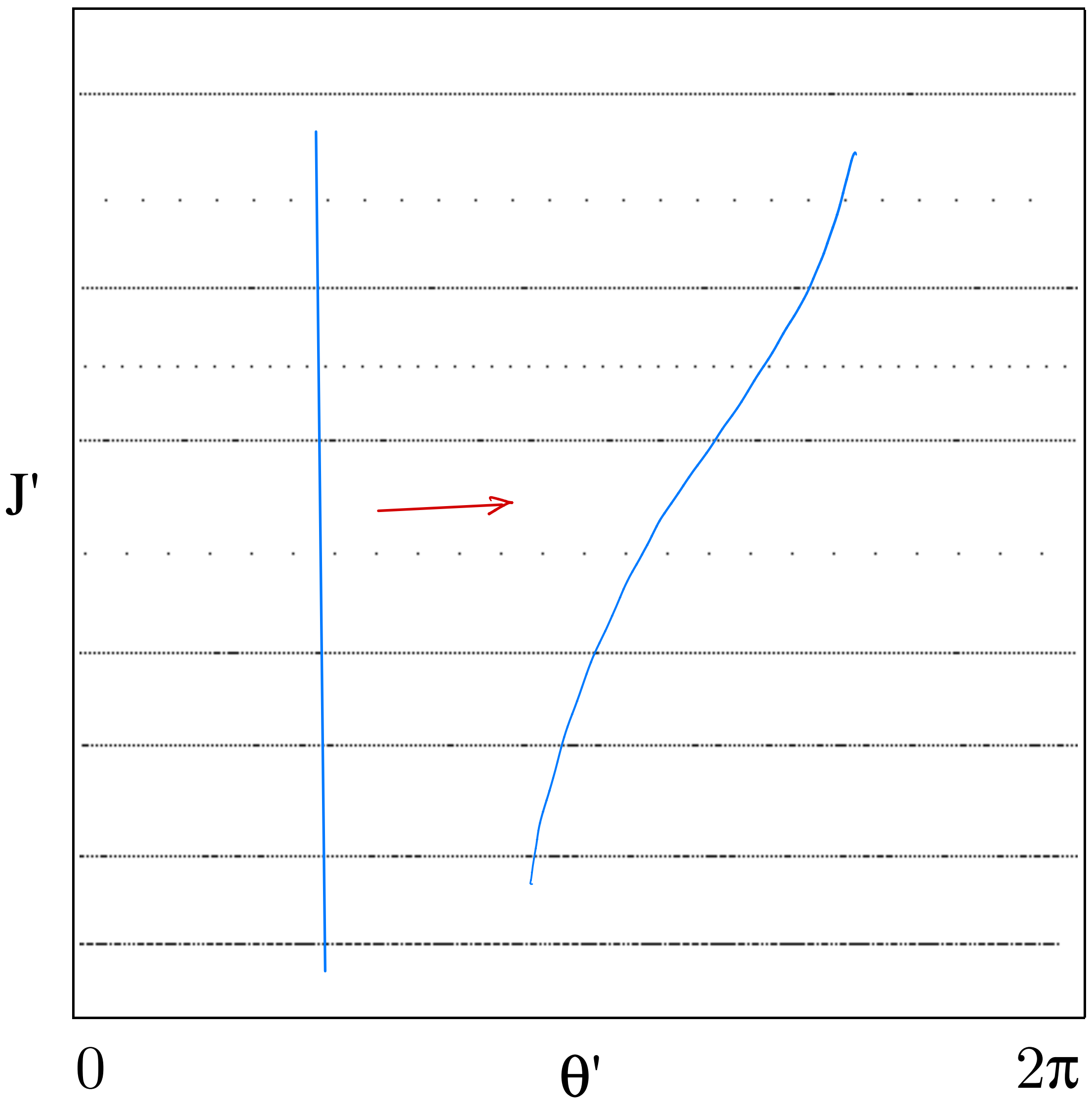


Integrable Symplectic (area preserving) Map

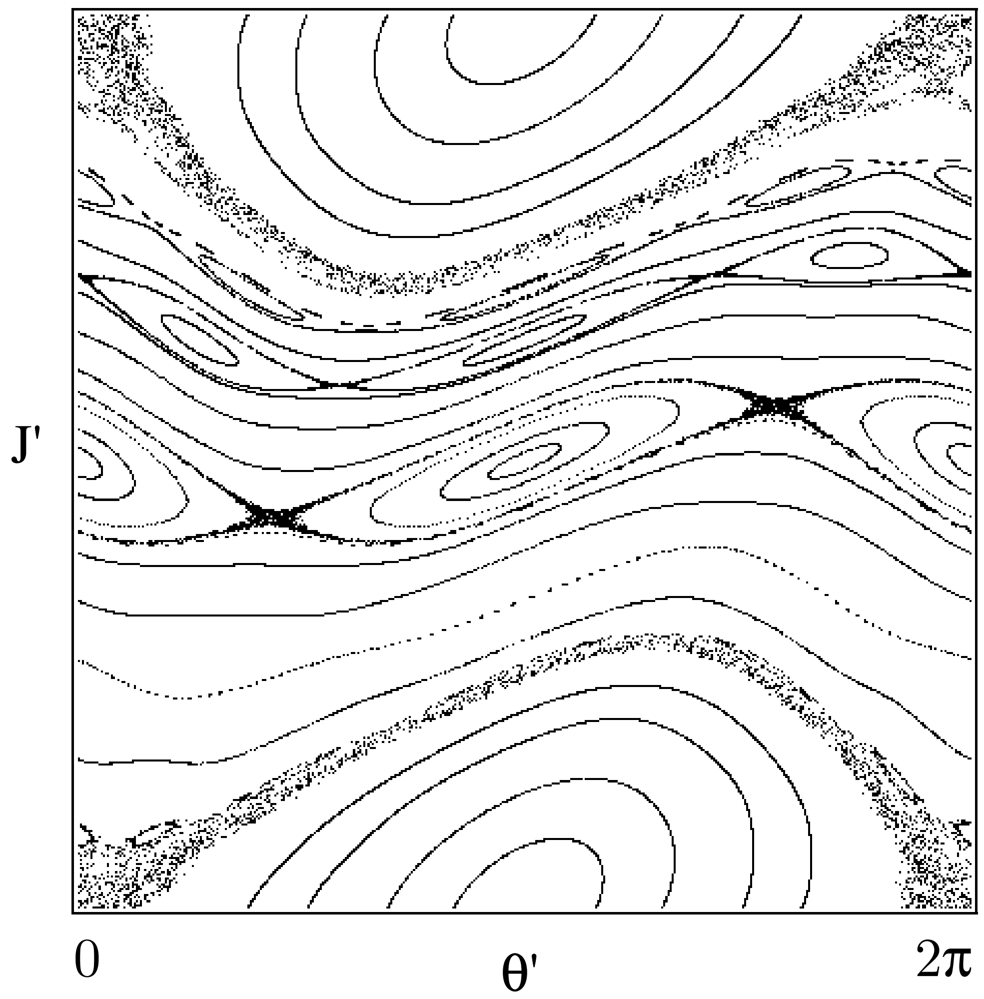




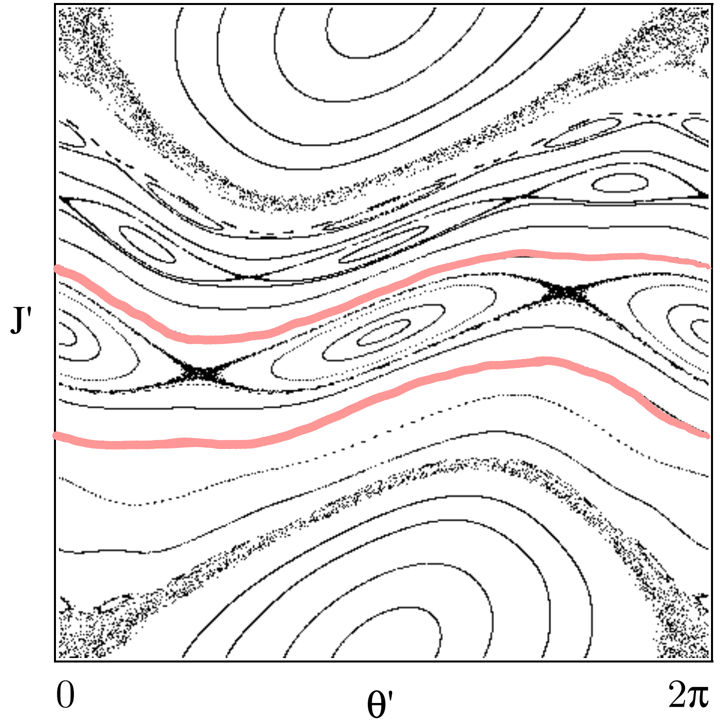
Integrable Symplectic **Twist** Map (Moser)



Nonintegrable Symplectic Map (imperfect coils and/or plasma response)



Nonintegrable Symplectic **Twist** Map



Poincaré-Birkhoff: area-preserving, orientation-preserving homeomorphism of an annulus with boundaries rotating at different rates has an even number of fixed points, half stable and half unstable.

Invariant circle preservation and island physics are very important in plasma confinement.

The Standard Map ← Universality

Chirikov & Greene: $M : \mathbb{T} \times \mathbb{R} \to \mathbb{T} \times \mathbb{R}$

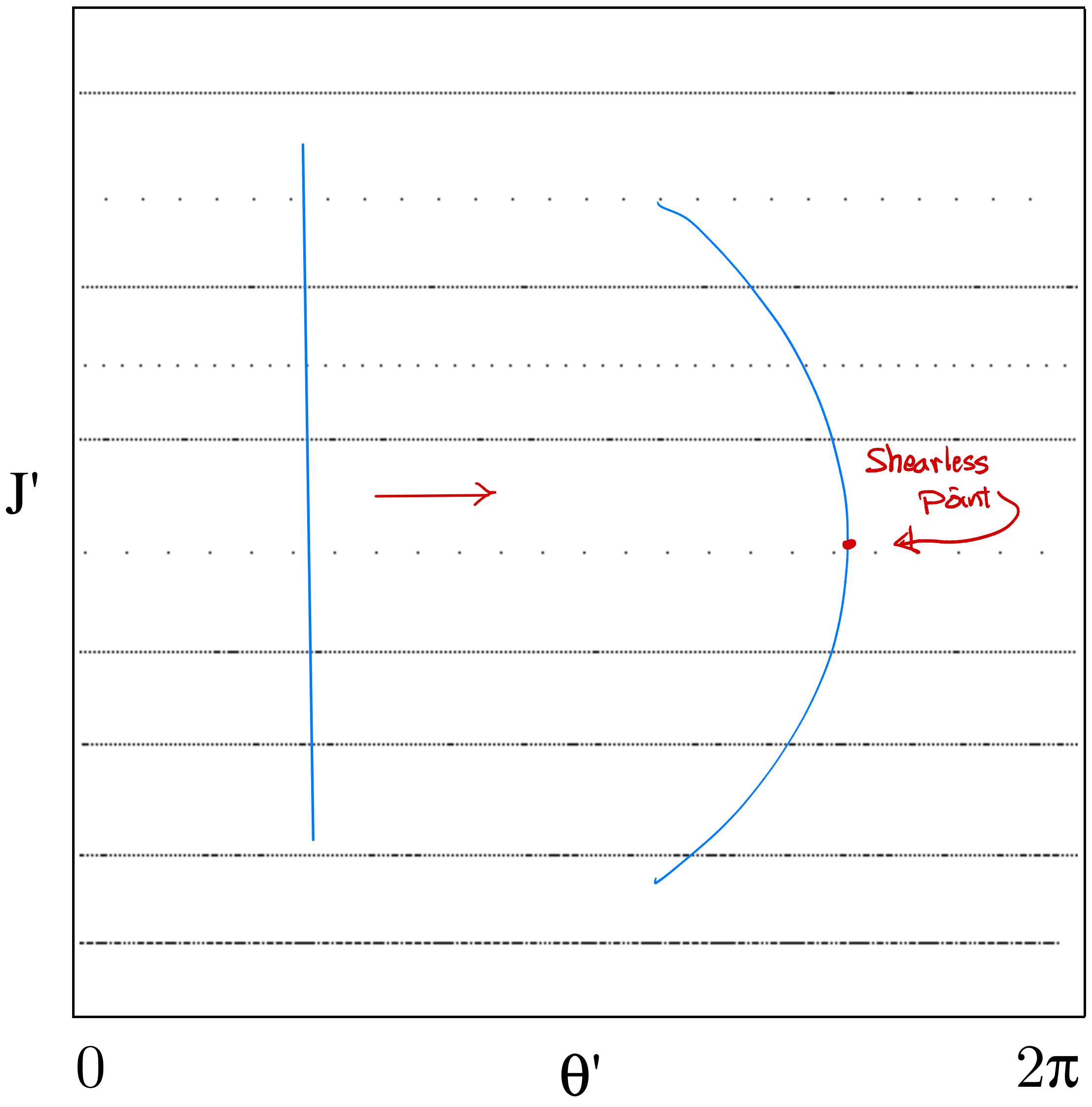
$$\begin{aligned} \bar{x} &= x + \bar{y}, \qquad mod\ 1 \\ \bar{y} &= y + k \sin(2\pi x) \end{aligned}$$

Circles with rotation number having continued fraction expansion $[\ldots, 1, 1, 1, \ldots]$ (noble numbers). For the standard map, last to go has rotation number γ^{-1}, Greene calculated to many places 0.971635406. Circle breaks like a phase transition & $\exists$ universal scaling number.

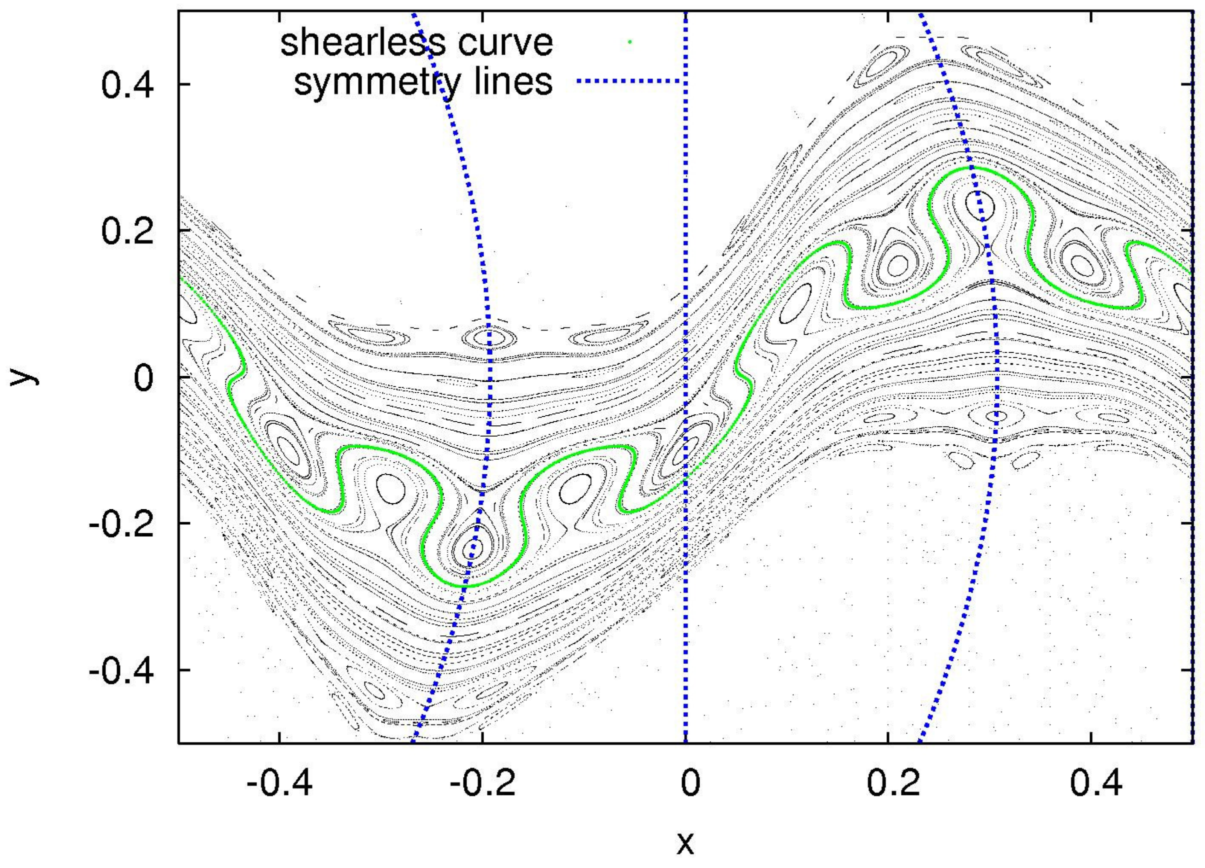
Wilbrink & others: $\sin(2\pi) \to \mathrm{saw}(x) \in C^0(\mathbb{T})$ defined by

$$\mathrm{saw}(x) = \begin{cases} 4x & 0 \leq x < 1/4 \\ 4(1/2 - x) & 1/4 \geq x < 3/4 \\ 4(-1 + x) & x \geq 3/4 \end{cases}$$

Integrable Symplectic **Nonwist** Map



Nonintegrable Symplectic **Nonwist** Map



The Standard Nontwist Map $\leftarrow$ Universality

del-Castillo & pjm:

$$\bar{x} = x + a(1 - \bar{y}^2) \qquad mod\ 1$$
$$\bar{y} = y - b\,\sin(2\pi x)$$

Shearless circles with noble rotation numbers are sturdy. It is codimension two with two universal scaling exponents.

See e.g. pjm & A. Wurm, Scholarpedia article for many references.

II. Flows on Poisson manifolds

Sophus Lie (1890) $\longrightarrow$ Lichnerowicz, Sudarshan, Arnold $\longrightarrow$ PJM & Greene (1980, noncanonical) $\longrightarrow$ A. Weinstein (1983, Poisson Manifolds etc.) $\longrightarrow$ . . .

Noncanonical Poisson Brackets – Flows on Poisson Manifolds

Definition. A Poisson manifold $\mathcal{Z}$ has bracket

$$\{\,,\,\}\colon C^\infty(\mathcal{Z}) \times C^\infty(\mathcal{Z}) \to C^\infty(\mathcal{Z})$$

st $C^\infty(\mathcal{Z})$ with $\{\,,\,\}$ is a Lie algebra realization, i.e., is

- $\mathbb{R}$-bilinear,
- antisymmetric,
- Jacobi identity
- Leibniz, i.e., acts as a derivation $\Rightarrow$ vector field.

Geometrically $C^\infty(\mathcal{Z}) \equiv \Lambda^0(\mathcal{Z})$ and $\boldsymbol{d}$ exterior derivative.

$$\{f,g\} = \langle \boldsymbol{d}f, J\boldsymbol{d}g\rangle = J(\boldsymbol{d}f, \boldsymbol{d}g) = \frac{\partial f}{\partial z^i} J^{ij} \frac{\partial g}{\partial z^j}\,.$$

J the Poisson tensor/operator. Flows are integral curves of noncanonical Hamiltonian vector fields, $J\boldsymbol{d}H$, i.e.,

$$\dot{z}^i = J^{ij}(z)\frac{\partial H(z)}{\partial z^j}\,, \qquad \mathcal{Z}'s \text{ coordinate patch } z = (z^1, \ldots, z^N)$$

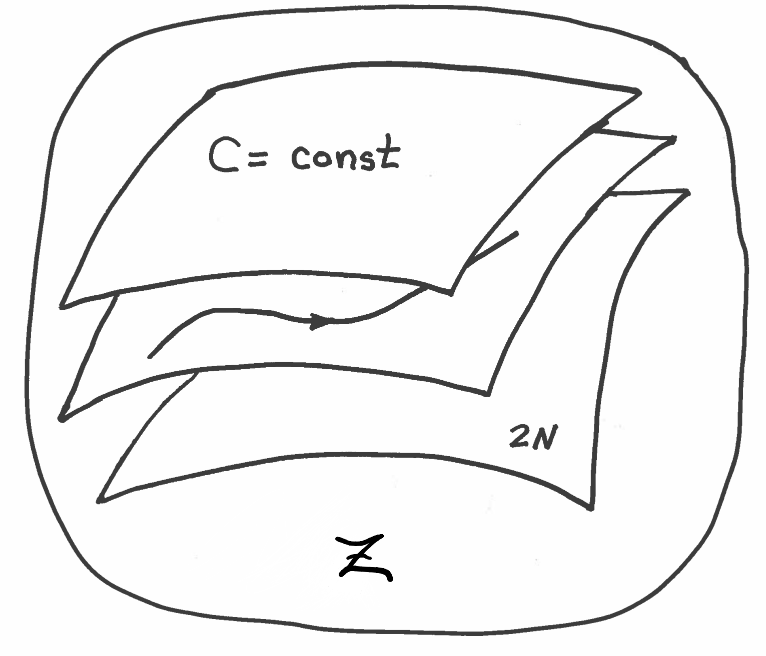
Because of degeneracy, $\exists$ functions C st $\{f, C\} = 0$ for all $f \in C^\infty(\mathcal{Z})$, called Casimir invariants (Lie's distinguished functions!).

Poisson Manifold (phase space) $\mathcal{Z}$ Cartoon

Degeneracy in J $\Rightarrow$ Casimirs:

$$\{f, C\} = 0 \quad \forall\ f : \mathcal{Z} \to \mathbb{R}$$

Lie-Darboux Foliation by Casimir (symplectic) leaves:



Lie-Poisson Brackets

$\mathfrak{g}$ a dim-n Lie algebra with basis $\{e_i\}_{i=1}^n$ and structure constants $\{c_{ij}^k\}$, i.e., $[e_i, e_j] = c_{ij}^k e_k$

$\mathfrak{g}^*$ dual algebra with pairing $\langle\cdot,\cdot\rangle\colon \mathfrak{g}^*\times\mathfrak{g}\to\mathbb{R}$ and basis $\{e_*^i\}_{i=1}^n$ st $\langle e_*^i, e_j\rangle = \delta_j^i$

For smooth $f\colon \mathfrak{g}^*\to\mathbb{R}$, $\boldsymbol{d}f(\mu)\in\mathfrak{g}$ evaluated at $\mu\in\mathfrak{g}^*$ for any $\delta\mu\in\mathfrak{g}^*$,

$$\frac{d}{ds}f(\mu+s\delta\mu)\Big|_{s=0}\langle\delta\mu,\boldsymbol{d}f(\mu)\rangle \qquad \to \qquad \boldsymbol{d}f(\mu)=\frac{\partial f}{\partial\mu_i}(\mu)\,e_i.$$

Lie–Poisson bracket for any $f, g\colon \mathfrak{g}^*\to\mathbb{R}$ is

$$\{f,g\}_{\mathfrak{g}}(\mu) := \langle\mu,[\boldsymbol{d}f(\mu),\boldsymbol{d}g(\mu)]\rangle = \mu_k c_{ij}^k\frac{\partial f}{\partial\mu_i}\frac{\partial g}{\partial\mu_j}. \qquad (1)$$

Lie–Poisson dynamics for a Hamiltonian $H\colon \mathfrak{g}^*\to\mathbb{R}$ is given by

$$\dot\mu_i = \{\mu_i, H\}_{\mathfrak{g}} = \mu_k c_{ij}^k\frac{\partial H}{\partial\mu_j}, \qquad \Leftrightarrow \qquad \dot\mu = -\,\mathrm{ad}^*_{\boldsymbol{d}h(\mu)}\,\mu. \qquad (2a)$$

Clebsch Canonization (pjm 1980, Jayawardana et al. 2022)

Associated with Lie–Poisson bracket $\exists$ special canonical system for $\bar{f}, \bar{g} \colon T^*\mathbb{R}^n \to \mathbb{R}$:

$$\{\bar{f}, \bar{g}\} = \frac{\partial \bar{f}}{\partial q^i}\frac{\partial \bar{g}}{\partial p_i} - \frac{\partial \bar{g}}{\partial q^i}\frac{\partial \bar{f}}{\partial p_i},$$

where $\mu = \mu_i e^i_* \in \mathfrak{g}^*$ and $(q, p) \in T^*\mathbb{R}^n$ are related as follows:

$$\mu_i = c^k_{ij} q^j p_k.$$

$f, g \colon \mathfrak{g}^* \to \mathbb{R}$, we define $\bar{f}, \bar{g} \colon T^*\mathbb{R}^n \to \mathbb{R}$ by $\bar{f}(q, p) := f(\mu)$. Then the chain rule $\Rightarrow$

$$\frac{\partial \bar{f}}{\partial q^i} = \frac{\partial f}{\partial \mu_j}\frac{\partial \mu_j}{\partial q^i} = \frac{\partial f}{\partial \mu_j} c^k_{ji} p_k, \qquad \frac{\partial \bar{f}}{\partial p_i} = \frac{\partial f}{\partial \mu_j}\frac{\partial \mu_j}{\partial p_i} = \frac{\partial f}{\partial \mu_j} c^i_{jk} q^k$$

using the Jacobi identity $\Rightarrow$

$$\{\bar{f}, \bar{g}\}(q, p) = \frac{\partial \bar{f}}{\partial q^i}\frac{\partial \bar{g}}{\partial p_i} - \frac{\partial \bar{g}}{\partial q^i}\frac{\partial \bar{f}}{\partial p_i} = \mu_i c^i_{jk} \frac{\partial f}{\partial \mu_j}\frac{\partial g}{\partial \mu_k} = \{f, g\}_{\mathfrak{g}}(\mu),$$

If the canonical system is solved with Hamiltonian $\bar{H}(q, p) = H(\mu)$ for $(q(t), p(t))$, then $\mu(t)$ solves the Lie–Poisson system!

Poisson Integrator

Def. A Poisson integrator exactly preserves symplectic leaves and is symplectic on leaf.

Thm. *For a class of Lie algebras, a symplectic integrator on* $T^*\mathbb{R}^n$ is Poisson on $\mathfrak{g}^*$.

Comment. Although the dimension is doubled, $\exists$ invariants on $T^*\mathbb{R}^n$ that make it efficient. (dual moment maps)

The Kida Vortex

The Kida vortex is an elliptical patch of constant vorticity in a two-dimensional Euler fluid flow. Dynamical variables are the semi axes a, b and the angle ϕ of orientation:

$$\dot{a} = \frac{\epsilon}{2} a \sin(2\phi), \qquad \dot{b} = -\frac{\epsilon}{2} b \sin(2\phi), \qquad \dot{\phi} = \frac{ab}{(a+b)^2} + \frac{\omega}{2} + \frac{\epsilon}{2}\frac{a^2+b^2}{a^2-b^2}\cos(2\phi),$$

where $\epsilon > 0$ is strain of the background shear flow.

Kida is Lie-Poisson for $\mathfrak{so}(2,1)$ with basis

$$e_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \qquad e_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \qquad e_3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

structure constants satisfy, for any $\mu \in \mathfrak{so}(2,1)^* \cong \mathbb{R}^3$,

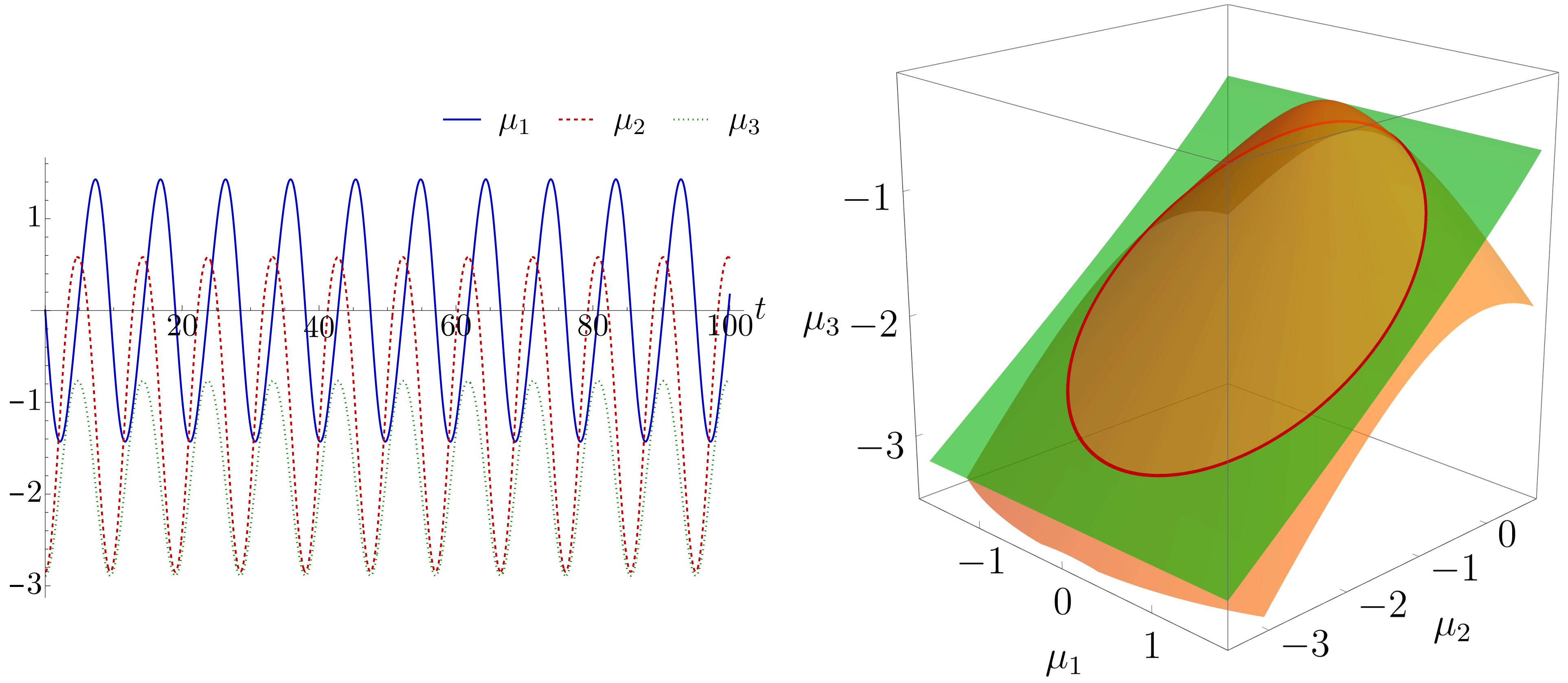
$$\mu_k c_{ij}^k = \begin{bmatrix} 0 & \mu_3 & \mu_2 \\ -\mu_3 & 0 & -\mu_1 \\ -\mu_2 & \mu_1 & 0 \end{bmatrix}.$$

This algebra has the Casimir

$$C(\mu) := \mu_1^2 + \mu_2^2 - \mu_3^2,$$

which is essentially the area of the ellipse.

Poisson Integration for Kida



(Left) Time evolution of μ $0 \leq t \leq 100$ with time step $\Delta t = 0.1$. μ using the canonized system. (right) Red curve is the Lie–Poisson dynamics in $\mathfrak{g}^* = \mathfrak{so}(2,1)^* \cong \mathbb{R}^3$ computed using the canonized system and momentum mapped by. Green and orange surfaces are the level sets of the Hamiltonian H and the Casimir C.

Why Poisson Integrator?

• Important classical systems have noncanonical Poisson brackets:

Magnetohydrodynamics pjm & Greene (1980),

Maxwell – Vlasov system (1980, 1982), Marsden & Weinsten (1982)

BBGKY heirarchy: Marsden, pjm, &Weinsetin (1984)

...

GEMPIC, a particle-in-cell (PIC) code Kraus et. al (2017). FEEC builds De Rham cohomology into numerics for Maxwell's equations etc.

III. Metriplectic Dynamics

Theory of thermodynamically consistent theories

Theory = Dynamical System = $\mathfrak{X}(\mathcal{Z})$

Finite dimensions $\exists$ rigor. Infinite dimensions $\exists$ wishful thinking.

Circa 1980, Kaufman & pjm (1982), **pjm (1984, 1986)**, pjm & Hazeltine (1984), Grmela (1984), . . .

Fluid Mechanics Examples

Navier-Stokes is **inconsistent:**

$$\partial_t \boldsymbol{v} = -\boldsymbol{v}\cdot\nabla\boldsymbol{v} - \frac{1}{\rho_0}\nabla p + \nu\nabla^2\boldsymbol{v}\,, \qquad \nabla\cdot\boldsymbol{v} = 0 \quad \Rightarrow \quad p[\boldsymbol{v}]$$

$$H = \int_\Omega \rho_0\,|\boldsymbol{v}|^2/2 \quad \text{and} \quad \dot{H} \le 0\,, \quad \nexists \text{ any thermodynamics!}$$

Navier-Stokes-Fourier (NSF) is **consistent:** (Eckart 1940):

$$\partial_t \boldsymbol{v} = -\boldsymbol{v}\cdot\nabla\boldsymbol{v} - \frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla\cdot\mathcal{T} \qquad \text{viscous stress tensor is } \mathcal{T}$$

$$\partial_t \rho = -\nabla\cdot(\rho\boldsymbol{v})$$

$$\partial_t s = -\boldsymbol{v}\cdot\nabla s - \frac{1}{\rho T}\nabla\cdot\boldsymbol{q} + \frac{1}{\rho T}\mathcal{T}:\nabla\boldsymbol{v} \qquad \text{heat flux \& viscous heating}$$

$$H = \int_\Omega \rho\,|\boldsymbol{v}|^2/2 + \rho u(\rho, s)\,, \quad \dot{H} = 0 \quad \text{and} \quad S = \int_\Omega \rho s \;\to\; \dot{S} \ge 0$$

Example of Thermodynamic Completion, i.e. NS $\to$ NSF.

Thermodynamic Consistency

The realization in a **dynamical system** of the first and second laws of thermodynamics:

First Law is energy conservation:

$$\dot{H} = 0$$

Second Law is entropy production:

$$\dot{S} \geq 0$$

Good models lift thermodynamics to **dynamical systems.** They have two functions H, S.

Metriplectic Dynamics

Metric ∪ Symplectic Flows (pjm 1986) $\longleftrightarrow V_D + V_H \in \mathfrak{X}(\mathcal{Z})$

- Formalism for natural split of vector fields $\dot{z} = \{z, H\} + (z, S) = J\nabla H + G\nabla S$

- Enforces thermodynamic consistency: $\dot{H} = 0$ the 1st Law and $\dot{S} \geq 0$ the 2nd Law.

- Other invariants? E.g., collision operators preserve, mass, momentum, ... There exists some theory for building in, but won't discuss today.

- **Encompassing 4-bracket**: Entropy is a Casimir is & "curvature" is dissipation rate

Ideas of Casimirs are candidates for entropy, multibracket, curvature, etc. in pjm (1984). Metriplectic in pjm (1986).

What is Dissipation?

- Not all conservative systems are Hamiltonian
- Not all Hamiltonian systems are conservative
- Not all reversible systems are Hamiltonian
- All finite dynamical systems (autonomous ODEs) are reversible (1 parameter Lie group)
- Some infinite systems (PDEs) are reversible and some irreversible (group vs. semigroup)
- Not all Hamiltonian systems have time reversal symmetry
- Not all systems with time reversal symmetry are Hamiltonian
- $\exists$ systems with time reversible symmetry and global asymptotic stability

Thermodynamically Consistent Dissipation:
<u>Energy conserving</u> systems with an <u>increasing entropy</u> that implies <u>global asymptotic stability</u>.

Such systems have a 'vector field' that naturally splits in Hamiltonian and dissipative parts. Hamiltonian is an unambiguous way to define nondissipative. The <u>metriplectic 4-bracket</u> is an unambiguous way to define dissipative. Together they $\Rightarrow$ thermodynamic consistency.

Metriplectic 4-Bracket Dynamics

Dynamical System (finite or infinite):

$$\dot{z} = \{z, H\} + (z, H; S, H)$$

Dynamics for any observable (functional of dynamical variables), z, is generated by multilinear brackets, Poisson bracket + 4-bracket (2024), with Hamiltonian H and entropy = Casimir S.

Why a 4-Bracket?

- One slot for dynamical variables (observables), z.

- Two slots for two fundamental functions: Hamiltonian, H, and Entropy (Casimir), S.

- There remains one slot for $\mathcal{F}$, free energy like generator $\mathcal{F} = H - TS$. Better argument: Needed to have multilinearity.

Comments:

- Provides natural reductions to other bilinear & binary brackets.

- The three slot brackets of pjm 1984 were not trilinear. Four needed to be multilinear.

The Metriplectic 4-Bracket

4-bracket on 0-forms (functions):

$$(\,\cdot\,,\,\cdot\,;\,\cdot\,,\,\cdot\,)\colon \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \to \Lambda^0(\mathcal{Z})$$

For functions $f, k, g, n \in \Lambda^0(\mathcal{Z})$ in a coordinate patch the 4-bracket has the form:

$$(f, k; g, n) = R^{ijkl}(z)\frac{\partial f}{\partial z^i}\frac{\partial k}{\partial z^j}\frac{\partial g}{\partial z^k}\frac{\partial n}{\partial z^l}\,. \qquad \leftarrow \text{quadravector?}$$

• Metriplectic manifolds have both Poisson tensor, J^{ij}, and compatible quadravector R^{ijkl}, where S (selected from set of Casimirs) and H comes from Hamiltonian part.

A blend of my previous early ideas 1980s: Two important functions H and S, symmetries, curvature idea, multi-brackets.

Metriplectic 4-Bracket Properties

(i) $\mathbb{R}$-linearity in all arguments, e.g, for $\lambda \in \mathbb{R}$

$$(f + \lambda h, k; g, n) = (f, k; g, n) + \lambda(h, k; g, n)$$

(ii) algebraic identities/symmetries

$$(f, k; g, n) = -(k, f; g, n)\,, \qquad (f, k; g, n) = -(f, k; n, g)\,, \qquad (f, k; g, n) = (g, n; f, k)$$

(iii) derivation in all arguments, e.g.,

$$(fh, k; g, n) = f(h, k; g, n) + (f, k; g, n)h$$

where as usual, fh denotes pointwise multiplication.

Symmetries of algebraic curvature without torsion identity. **Minimal Metriplectic.**

Observation: Often see $R^l{}_{ijk}$ or R_{lijk} but not R^{lijk}! Never 4-bracket, i.e. action on 1-forms?

Properties – Existence – General Construction Methods

- Thermodynamic Consistency Built-in:

$$\dot{H} = \{H, H\} + (H, H; S, H) = 0 \qquad \text{and} \qquad \dot{S} = (S, H; S, H) \geq 0$$

Reduces to metriplectic 2-bracket (1984): $(F, G)_H = (F, H; G, H)$.

- For any Riemannian manifold ∃ metriplectic 4-bracket. This means there is a wide class of them, but the bracket tensor does not need to come from Riemann tensor only needs to satisfy the bracket properties.

- If Riemannian, entropy production rate is positive contravariant sectional curvature. For closed $\sigma, \eta \in \Lambda^1(\mathcal{Z})$, entropy production by

$$\dot{S} = K(\sigma, \eta) := (S, H; S, H) \geq 0\,,$$

where the second equality follows from $\sigma = \boldsymbol{d}S$ and $\eta = \boldsymbol{d}H$.

- Two methods of construction? **Kulkarni-Nomizu** (K-N) product and **Lie algebra** based. $K(\sigma, \eta) \geq 0$ automatic for K-N and easily made minimally degenerate!

Methods of Construction

Construction via Kulkarni-Nomizu Product

Given σ and μ, two symmetric rank-2 tensor fields operating on 1-forms (assumed exact) $\boldsymbol{d}f, \boldsymbol{d}k$ and $\boldsymbol{d}g, \boldsymbol{d}n$, the K-N product is

$$\begin{aligned}\sigma \owedge \mu\, (\boldsymbol{d}f, \boldsymbol{d}k, \boldsymbol{d}g, \boldsymbol{d}n) &= \sigma(\boldsymbol{d}f, \boldsymbol{d}g)\, \mu(\boldsymbol{d}k, \boldsymbol{d}n) - \sigma(\boldsymbol{d}f, \boldsymbol{d}n)\, \mu(\boldsymbol{d}k, \boldsymbol{d}g) \\ &+ \mu(\boldsymbol{d}f, \boldsymbol{d}g)\, \sigma(\boldsymbol{d}k, \boldsymbol{d}n) - \mu(\boldsymbol{d}f, \boldsymbol{d}n)\, \sigma(\boldsymbol{d}k, \boldsymbol{d}g)\, .\end{aligned}$$

Metriplectic 4-bracket:

$$(f, k; g, n) = \sigma \owedge \mu(\boldsymbol{d}f, \boldsymbol{d}k, \boldsymbol{d}g, \boldsymbol{d}n)\, .$$

In coordinates:

$$R^{ijkl} = \sigma^{ik}\mu^{jl} - \sigma^{il}\mu^{jk} + \mu^{ik}\sigma^{jl} - \mu^{il}\sigma^{jk}\, .$$

If σ or μ defines inner product, then minimally degenerate, one fixed point on $H=$ constant.

Infinite dimensions lift to operators: $\mu \to M\, , \quad \sigma \to \Sigma$.

Lie Algebra Based Metriplectic 4-Brackets

- For structure constants ${c^{kl}}_s$:

$$(f,k;g,n) = {c^{ij}}_r {c^{kl}}_s \, g^{rs} \frac{\partial f}{\partial z^i}\frac{\partial k}{\partial z^j}\frac{\partial g}{\partial z^k}\frac{\partial n}{\partial z^l}\,.$$

Lacks cyclic symmetry, but $\exists$ procedure to remove torsion (Bianchi identity) for any symmetric 'metric' g^{rs}. Dynamics does not see torsion, but manifold does.

- For $g^{rs}_{CK} = {c^{rl}}_k \, {c^{sk}}_l$ the Cartan-Killing metric, torsion vanishes automatically. Completely determined by Lie algebra. For $\mathfrak{so}(3)$ reproduces relaxing free rigid body (pjm 1986).

- Covariant connection $\nabla\colon \mathfrak{X}\times\mathfrak{X}\to\mathfrak{X}$. Instead, a contravariant connection on any Poisson manifold $D\colon \Lambda^1(\mathcal{Z})\times\Lambda^1(\mathcal{Z})\to\Lambda^1(\mathcal{Z})$ that satisfies Koszul identities, but Leibniz becomes $D_\alpha(f\gamma) = fD_\alpha\gamma + J(\alpha)[f]\gamma$ where $J(\alpha)[f] = \alpha_i J^{ij}\partial f/\partial z^j$ is a 0-form that replaces the term $\mathbf{X}(f)$ (Fernandes, 2000). Here $\alpha,\beta,\gamma\in\Lambda^1(\mathcal{Z})$, $f\in\Lambda^0(\mathcal{Z})$. Build 4-bracket like curvature from connection $\Rightarrow$?

Unified Thermodynamic (UT) Algorithm

UT Algorithm is an algorithm for constructing metriplectic systems! Akin to building Lagrangians. Applied to many systems. **So far UT Algorithm either reproduces, corrects, or extends for every case considered!**

Examples: Cahn-Hilliard-Navier-Stokes, Brenner-Navier-Stokes, Generalized Brenner-Navier-Stokes, generalization of Landau collision operator (thermo consistent nonlinear Fokker-Planck) ... .

Four Steps of the UT Algorithm

1. Identify dynamical variables defined on $\Omega \subset \mathbb{R}^3$; e.g. for NSF

$$\boldsymbol{\xi} = (\boldsymbol{m} = \rho \boldsymbol{v}, \rho, \sigma = \rho s)$$

2. Propose energy and entropy functionals, $H[\boldsymbol{\xi}]$ and $S[\boldsymbol{\xi}]$; for NSF

$$H = \int_\Omega \frac{|\mathbf{m}|^2}{2\rho} + \rho u(\rho, \sigma/\rho) \quad \text{and} \quad S = \int_\Omega \sigma$$

3. Find Poisson bracket $\{F, G\}$ for which entropy S is a Casimir invariant, $\{F, S\} = 0 \,\forall\, F$

4. Construct metriplectic 4-bracket $(F, K; G, N)$ via Kulkarni-Nomizu product. How? **We now have new method that separates local thermodynamics from phenomenological quantities**, giving the EoMs as Poisson bracket + 4-bracket:

$$\partial_t \boldsymbol{\xi} = \{\boldsymbol{\xi}, H\} + (\boldsymbol{\xi}, H; S, H)$$

Result automatically Thermodynamically consistent!

3. For NSF Ideal Fluid Poisson Bracket Dynamics

Hamiltonian:

$$H = \int_\Omega \frac{\rho|\mathbf{v}|^2}{2} + \rho u\,(\rho, s)\ , \qquad T = \frac{\partial u}{\partial s}\,, \qquad p = \rho^2 \frac{\partial u}{\partial \rho}\,.$$

Lie-Poisson Bracket (pjm-Greene, 1980):

$$\{F, G\} = -\int_\Omega \mathbf{m}\cdot[F_{\boldsymbol{m}}\cdot\nabla G_{\boldsymbol{m}} - G_{\boldsymbol{m}}\cdot\nabla F_{\boldsymbol{m}}] + \rho\,[F_{\boldsymbol{m}}\cdot\nabla G_\rho - G_{\boldsymbol{m}}\cdot\nabla F_\rho] + \sigma\,[F_{\boldsymbol{m}}\cdot\nabla G_\sigma - G_{\boldsymbol{m}}\cdot\nabla F_\sigma]\,.$$

Equations of Motion:

$$\partial_t \mathbf{v} = \{\boldsymbol{v}, H\} = -\boldsymbol{v}\cdot\nabla\boldsymbol{v} - \nabla p/\rho\,, \quad \partial_t\rho = \{\rho, H\} = -\nabla\cdot(\rho\,\boldsymbol{v})\,, \quad \partial_t\sigma = \{\sigma, H\} = -\nabla\cdot(\sigma\,\boldsymbol{v})\,.$$

Casimir:

$$S = \int_\Omega \rho s = \int_\Omega \sigma\,.$$

Note: $F_{\boldsymbol{m}} = \delta F/\delta \boldsymbol{m}$, etc., functional derivatives.

4. Metriplectic 4-Bracket

Old method (early 2024): guess the K-N quantities M and Σ.

New Method

Theorem: Order dynamical variables st

$$\partial_t \xi^\alpha = \{\xi^\alpha, H\} + \nabla \cdot \boldsymbol{J}^\alpha\,, \qquad\qquad \alpha = 1, \ldots, N-1\,,$$
$$\partial_t \xi^N = \{\xi^N, H\} + \nabla \cdot \boldsymbol{J}^N + \boldsymbol{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \boldsymbol{Z}_\beta\,.$$

where $\xi^N = \sigma$, the entropy density. Above splits Hamiltonian and conservative.

Then

$$\dot{S} = \int_\Omega \boldsymbol{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \boldsymbol{Z}_\beta =: \int_\Omega \dot{\sigma}^{prod} \geq 0\,.$$

and $\dot{H} \Rightarrow$

$$\boldsymbol{Z}_\alpha = \nabla H_{\xi^\alpha}\,, \qquad \boldsymbol{J}^\alpha = -H_{\xi^N} \tilde{L}^{\alpha\beta} \nabla H_{\xi^\beta} = -L^{\alpha\beta} \nabla H_{\xi^\beta}\,.$$

which leads naturally to

$$M(dF, dG) = F_{\xi^N} G_{\xi^N}\,, \qquad \Sigma(dF, dG) = \nabla(F_{\xi^\alpha}) \frac{L^{\alpha\beta}}{H_{\xi^N}} \nabla(G_{\xi^\beta})\,.$$

Important By-Product of UT Algorithm

- Special **ordering of dynamical variables** and concomitant 'Force-Flux' relations of nonequilibrium thermodynamics:

$$\boldsymbol{J}^{\alpha} = L^{\alpha\beta} X_{\beta} \quad \rightarrow \quad \boldsymbol{J}^{\alpha} = -L^{\alpha\beta}\, \nabla(\delta H/\delta\xi^{\beta})$$

'Forces': $\boldsymbol{X} \sim \nabla T, \nabla p, \nabla \boldsymbol{v}$ etc., UT Algorithm removes ambiguous selection of forces and provides definition of phenomenological coefficients, $L^{\alpha\beta}$, for dynamical variables ξ^{β}.

- Separates dependences on thermodynamical variables that come from internal energy U (local thermodynamic equilibrium) from those that appear in the phenomenological coefficients $L^{\alpha\beta}$. For example in in the Fourier heat law entropy production expression

$$\dot{\sigma}^{prod} = \nabla T \cdot \frac{\bar{\kappa}}{T^2} \cdot \nabla T$$

one T comes from Fourier's law $q = -\bar{\kappa}\nabla T/T$ while the other comes from the phenomenological coefficient.

- Physically identify the sectional curvature

$$\dot{S} = (S, H; S, H) = K(H, S) = \int_{\Omega} \Sigma(dH, dH) = \int_{\Omega} \nabla H_{\xi^{\alpha}} \cdot \tilde{L}^{\alpha\beta} \cdot \nabla H_{\xi^{\beta}} \geq 0\,.$$

4. Metriplectic 4-Bracket: General and NSF

General flux expressions:

$$\boldsymbol{J}_\rho = -L^{\rho\rho}\cdot\nabla H_\rho - L^{\rho\boldsymbol{m}}:\nabla H_{\boldsymbol{m}} - L^{\rho\sigma}\cdot\nabla H_\sigma\,,$$
$$\bar{J}_{\mathbf{m}} = -L^{\boldsymbol{m}\rho}\otimes\nabla H_\rho - L^{\boldsymbol{m}\boldsymbol{m}}:\nabla H_{\boldsymbol{m}} - L^{\boldsymbol{m}\sigma}\otimes\nabla H_\sigma\,,$$
$$\boldsymbol{J}_\sigma = -L^{\sigma\rho}\cdot\nabla H_\rho - L^{\sigma\boldsymbol{m}}:\nabla H_{\boldsymbol{m}} - L^{\sigma\sigma}\cdot\nabla H_\sigma\,,$$

where $\boldsymbol{J}_\rho$ is mass flux, $\bar{J}_{\mathbf{m}}$ is momentum flux 2-tensor, and $\boldsymbol{J}_\sigma$ is entropy flux.

For **NSF** all zero except:

$$L^{\boldsymbol{m}\boldsymbol{m}} = \bar{\bar{\Lambda}} \quad \text{and} \quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T}\,.$$

$\bar{\bar{\Lambda}}$ isotropic 4-tensor, $\bar{\kappa}$ conduction 2-tensor

$$\dot{S} = (S,H;S,H) = \int_\Omega \Sigma(dH,dH) = \int_\Omega \nabla\mathbf{v} : \frac{\bar{\bar{\Lambda}}}{T} : \nabla\mathbf{v} + \nabla T\cdot\frac{\bar{\kappa}}{T^2}\cdot\nabla T \geq 0\,.$$

Note in $\bar{\kappa}/T^2$ one T from H one from $L^{\alpha\beta}$. Σ sectional curvature density?

4. Metriplectic 4-Bracket for NSF Generalizations

For **Brenner NSF** all zero except:

$$L^{m\rho} = \tilde{D}\rho\, \boldsymbol{m}\,, \quad L^{m\sigma} = \tilde{D}\hat{\sigma}\, \boldsymbol{m}\,, \quad L^{mm} = \bar{\bar{\Lambda}} + \tilde{D}\, \boldsymbol{m} \otimes \bar{I} \otimes \boldsymbol{m}\,.$$

$$L^{\sigma\rho} = \tilde{D}\rho\hat{\sigma}\, \bar{I}\,, \quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T} + \tilde{D}\hat{\sigma}^2\, \bar{I} \quad L^{\sigma m} = \tilde{D}\hat{\sigma}\, \bar{I} \otimes \boldsymbol{m}$$

$$\dot{S} = \int_\Omega \frac{1}{T}\left[\frac{\tilde{D}}{\kappa_T^2\rho^2}|\nabla\rho|^2 + \nabla T \cdot \frac{\bar{\kappa}}{T} \cdot \nabla T \ + \nabla \boldsymbol{v} : \bar{\bar{\Lambda}} : \nabla \boldsymbol{v}\right] \geq 0\,.$$

Generalization of Brenner by **Reddy et al.** (2019) falls out. We further generalized.

IV. Metriplectic Dynamics and Contact Hamiltonian Dynamics

Y-G Oh at SLMath

Contact Structures Hamiltonian Dynamics

Contact Manifold:
$(\mathcal{Z}, \lambda \in \Lambda^1)$ where $\mathcal{Z}$ dimension $2n+1$; vectors in $\ker\lambda$ maximally nonintegrable hyperplane field.

Darboux Coordinates:
$\lambda = dz - p \cdot dq \quad \rightarrow \quad d\lambda = -dp \wedge dq$

Reeb Vector Field:
$\lambda(R) = 1 \qquad \text{and} \qquad d\lambda(R, \cdot\,) = 0$

Reeb vector field is analog of Hamiltonian vector field.

Canonical Contact Hamiltonian System:

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q} - p\frac{\partial H}{\partial z}, \qquad \dot{z} = -H + p \cdot \frac{\partial H}{\partial p}$$

where $H(q, p, z)$

Contact Hamiltonian Dynamics Properties

Energy Dissipation:

$$\dot{H} = -H\frac{\partial H}{\partial z}$$

does not vanish unless $H = 0$ or $\partial H/\partial z = 0$. In general **not** thermodynamically consistent

Is entropy z?:

$$\dot{z} = L$$

In general has no definite sign, i.e., **not** a Lyapunov function, but could be?

Metriplectic Construction

Trivial Poisson Manifold:

$$\mathcal{Z} = T^*\mathbb{R}^n \times \mathbb{R} \qquad \leftarrow \qquad \text{stack of symplectic hyperplanes}$$

Darboux Coordinates:

$$J = \begin{bmatrix} 0_n & I_n & 0 \\ -I_n & 0_n & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Poisson bracket:

$$\{f, g\} = J(df, dg) \quad \text{for} \quad f, g \in \Lambda^0(\mathcal{Z})$$

Casimirs:

$$C = C(z) \qquad \leftarrow z \qquad \text{could be entropy}$$

Lie-Poisson Dynamics:

$$\begin{bmatrix} \dot{q} \\ \dot{p} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} 0_n & I_n & 0 \\ -I_n & 0_n & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \partial H/\partial q \\ \partial H/\partial p \\ \partial H/\partial z \end{bmatrix}.$$

Metriplectic 4-Bracket

Kulkarni-Nomizu product:

$$\mu(df, dg) = \frac{\partial f}{\partial z}\frac{\partial g}{\partial z} \qquad \text{and} \qquad \sigma(df, dg) = \frac{\partial f}{\partial p} \cdot \frac{\partial g}{\partial p}$$

Metriplectic 4-Bracket:

$$(f, k; g, n) = \frac{\partial f}{\partial p} \cdot \frac{\partial g}{\partial p}\frac{\partial k}{\partial z}\frac{\partial n}{\partial z} - \frac{\partial f}{\partial p} \cdot \frac{\partial n}{\partial p}\frac{\partial k}{\partial z}\frac{\partial g}{\partial z} + \frac{\partial k}{\partial p} \cdot \frac{\partial n}{\partial p}\frac{\partial f}{\partial z}\frac{\partial g}{\partial z} - \frac{\partial k}{\partial p} \cdot \frac{\partial g}{\partial p}\frac{\partial f}{\partial z}\frac{\partial n}{\partial z}$$

Metriplectic Dynamics:

$$\dot{q} = \{q, H\} + (q, H; S, H) = \frac{\partial H}{\partial p}$$

$$\dot{p} = \{q, H\} + (p, H; S, H) = -\frac{\partial H}{\partial q} - \frac{\partial H}{\partial p}\frac{\partial H}{\partial z}$$

$$\dot{z} = (z, H; S, H) = \left|\frac{\partial H}{\partial p}\right|^2 \geq 0$$

By construction $\dot{H} = 0$. It is thermodynamically consistent with entropy z.

Comparison with Contact Hamiltonian

$$
\begin{aligned}
\dot{q}^i &= \{q^i, H\} + (q^i, H; S, H) = \frac{\partial H}{\partial p_i} = \frac{\partial H}{\partial p_i} \\
\dot{p}_i &= \{p_i, H\} + (p_i, H; S, H) = -\frac{\partial H}{\partial q^i} - \frac{\partial H}{\partial p^i}\frac{\partial H}{\partial z} \neq -\frac{\partial H}{\partial q^i} - p_i\frac{\partial H}{\partial z} \\
\dot{z} &= (z, H; S, H) = \left|\frac{\partial H}{\partial p}\right|^2 \neq -H + p \cdot \frac{\partial H}{\partial p}\,.
\end{aligned}
$$

Not the same. **Unless**, H Euler homogeneous of degree 2, e.g., geodesic

$$H = g(p,p)/2 = g^{ij} p_i p_j/2 = p_i p^i/2\,.$$

Comment: Open class of dynamical systems to study.

Final Comments on Metriplectic Dynmics

- Metriplectic dynamics is rich in geometry and produces interesting dynamical systems. Tons of interesting geometry already ... more to explore.

- The UT Algorithm based on the metriplectic 4-bracket, is a proven framework, provides a direct method for constructing thermodynamically consistent systems.

- Metriplectic Integrators: Metriplectic 4-brackets are easy to discretize while maintaining symmetries. First numerical implementation via 4-bracket discretization (Barham et al. 2025) for 1-D Navier-Stokes-Fourier. Finite element projection of PDE to thermodynamically consistent finite-dimensional 4-bracket, i.e., ODEs. For example, for the density $\rho(x,t)$

$$\rho_h(x,t) = \sum_{i=1}^{N} \rho_i(t)\phi_i(x) \quad \rightarrow \quad \dot{\rho}_i(t) = \{\rho_i, H\} + (\rho_i, H; S, H) \ldots$$

Results use Firedrake library, implicit midpoint, Irksome module ...

V. Final Comments

Overview

I. Symplectic maps

- Magnetic devices and zonal flows

II. Flows on finite-dimensional Poisson manifolds

- Symplectic and Clebsch-Poisson integrators – the Kida vortex.

III. Metriplectic Dynamics (thermodynamically consistent systems)

IV. Comparison of Metriplectic Dynamics to Contact Hamiltonian Dynamics

V. Final Comments