# I. Clebsch Lie-Poisson Integration, II. Simulated Annealing, and III. Metriplectic Relaxation

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# Poisson Brackets and Bracket Dissipation

Hamiltonian:

- Noncanonical Poisson Brackets (pjm 1980s) $\longleftarrow$ I.

Dissipation:

- Degenerate Antisymmetric Bracket (Kaufman and pjm, 1982)

- Double Brackets (Vallis, Carnevale, Bloch, ... 1989) $\longleftarrow$ II.

- Metriplectic Dynamics (pjm 1984,1986) $\longleftarrow$ III.

- Other 1984, Kaufman (no degeneracy), Grmela (no symmetry)

# I. Clebsch Lie-Poisson Integrator

# Noncanonical Hamiltonian Structure - Poisson Bracket Dynamics

Sophus Lie (1890) $\longrightarrow$ PJM (1980) $\longrightarrow$ Poisson Manifolds etc.

Noncanonical Coordinates:

$$\dot{z}^a = \{z^j, H\} = J^{ab}(z)\frac{\partial H}{\partial z^b}$$

Noncanonical Poisson Bracket:

$$\{A, B\} = \frac{\partial A}{\partial z^a} J^{ab}(z) \frac{\partial B}{\partial z^b}\,, \qquad \{\,,\}: C^\infty(\mathcal{Z}) \times C^\infty(\mathcal{Z}) \rightarrow C^\infty(\mathcal{Z})$$

Poisson Bracket Properties:

antisymmetry $\longrightarrow$ $\{A, B\} = -\{B, A\}$

Jacobi identity $\longrightarrow$ $\{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0$

Leibniz $\longrightarrow$ $\{AC, B\} = A\{C, B\} + \{C, B\}A$

G. Darboux: $detJ \neq 0 \Longrightarrow J \rightarrow J_c$ Canonical Coordinates

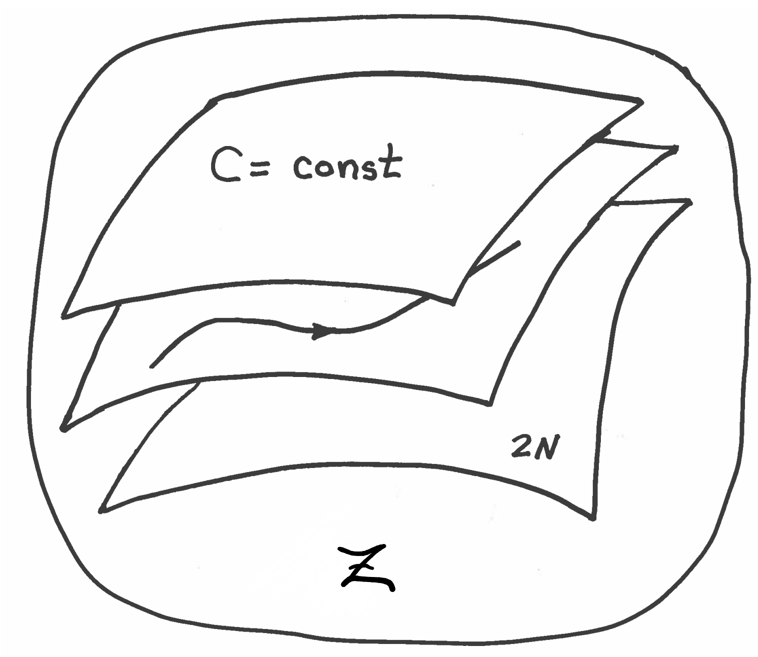
Sophus Lie: $detJ = 0 \Longrightarrow$ Canonical Coordinates plus Casimirs
(Lie's distinguished functions!)

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

Degeneracy in $J$ $\Rightarrow$ Casimirs:

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

Lie-Darboux Foliation by Casimir (symplectic) leaves:



## Poisson Integration

Symplectic integrators: time step with canonical transformation.

Poisson integrators: time step such that (i) symplectic on leaf and (ii) remains on leaf **exactly!**

* GEMPIC for the Vlasov equation: Kraus et al., J. Plasma Physics **83**, 905830401 (51pp) (2017).

* B. Jayawardana, P. J. Morrison, and T. Ohsawa, *Clebsch Canonization of Lie–Poisson Systems*, J. Geometric Mechanics **14**, 635–658 (2022).

# Lie-Poisson Brackets

Lie-Poisson brackets are special kind of noncanonical Poisson bracket that are associated with any Lie algebra, say $\mathfrak{g}$.

Natural phase space $\mathfrak{g}^*$. For $f, g \in C^\infty(\mathfrak{g}^*)$, $\mu \in \mathfrak{g}^*$, and $\mathbf{d}f \in \mathfrak{g}$,

Lie-Poisson bracket has the form

$$\begin{aligned} \{f, g\}_{LP} &= \langle \mu, [\mathbf{d}f, \mathbf{d}g]_{\mathfrak{g}} \rangle \\ &= \frac{\partial f}{\partial \mu_i} c^k{}_{ij}\, \mu_k \frac{\partial g}{\partial \mu_j}\,, \qquad\qquad i, j, k = 1, 2, \ldots, \dim \mathfrak{g} = n \end{aligned}$$

Pairing $<\ ,\ >$: $\mathfrak{g}^* \times \mathfrak{g} \to \mathbb{R}$, $\mu_i$ coordinates for $\mathfrak{g}^*$, and $c^{ij}{}_k$ structure constants of $\mathfrak{g}$.

# Lie-Poisson Brackets and Clebsch Canonization

"unreduction" pjm (1980), Clebsch 1859, **geometry new!**

Given Lie-Poisson system: $f, g \colon \mathfrak{g}^* \to \mathbb{R}$, coords $\mu$

Construct canonical system: $\bar{f}, \bar{g} \colon T^*\mathbb{R}^n \to \mathbb{R}$, coords $z = (q, p)$

Canonical Poisson Bracket: $\{\bar{f}, \bar{g}\}_c = \frac{\partial \bar{f}}{\partial q^i} \frac{\partial \bar{g}}{\partial p_i} - \frac{\partial \bar{g}}{\partial q^i} \frac{\partial \bar{f}}{\partial p_i}$

Poisson Map: $\boxed{\mu_i = c^k_{\ ij} q^j p_k}$

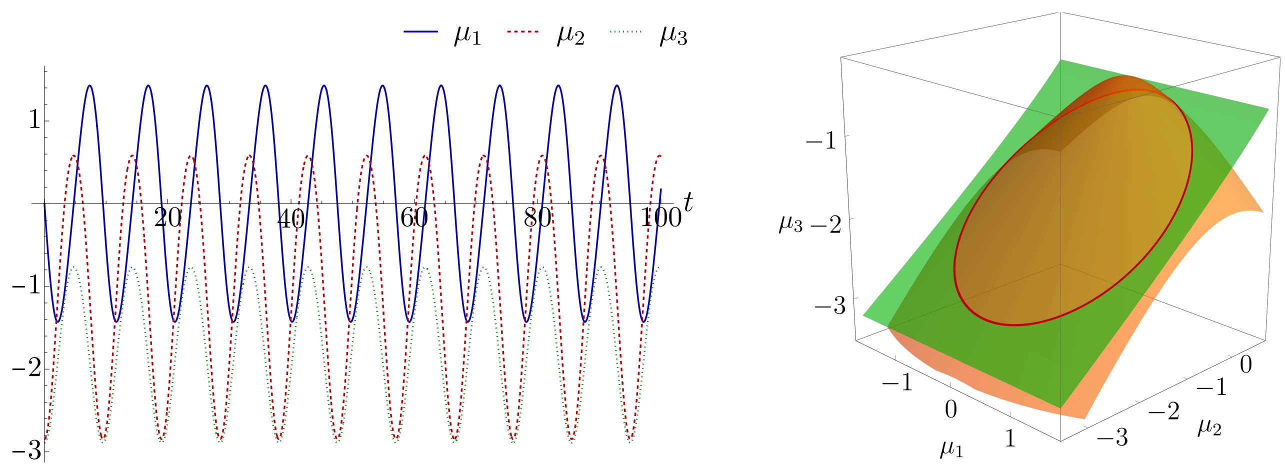
Momentum Map: $\{\bar{f}, \bar{g}\}_c = \{f, g\}_{LP}$, $\bar{H}(z) = H(\mu)$

$\exists$ Dual Pair – a second momentum map and invariants $\Rightarrow$

$\boxed{\text{Using symplectic Runge-Kutta on } T^*\mathbb{R}^n \Rightarrow \text{Poisson on } \mathfrak{g}^*!}$

# Example: Kida Vortex (nonseparable)

2D Euler Fluid, elliptical vortex patch, exact, Lie-Poisson with $\mathfrak{so}(2,1)$, Casimir $C = \mu_1^2 + \mu_2^2 - \mu_3^2$. (Meacham et al. 1997)

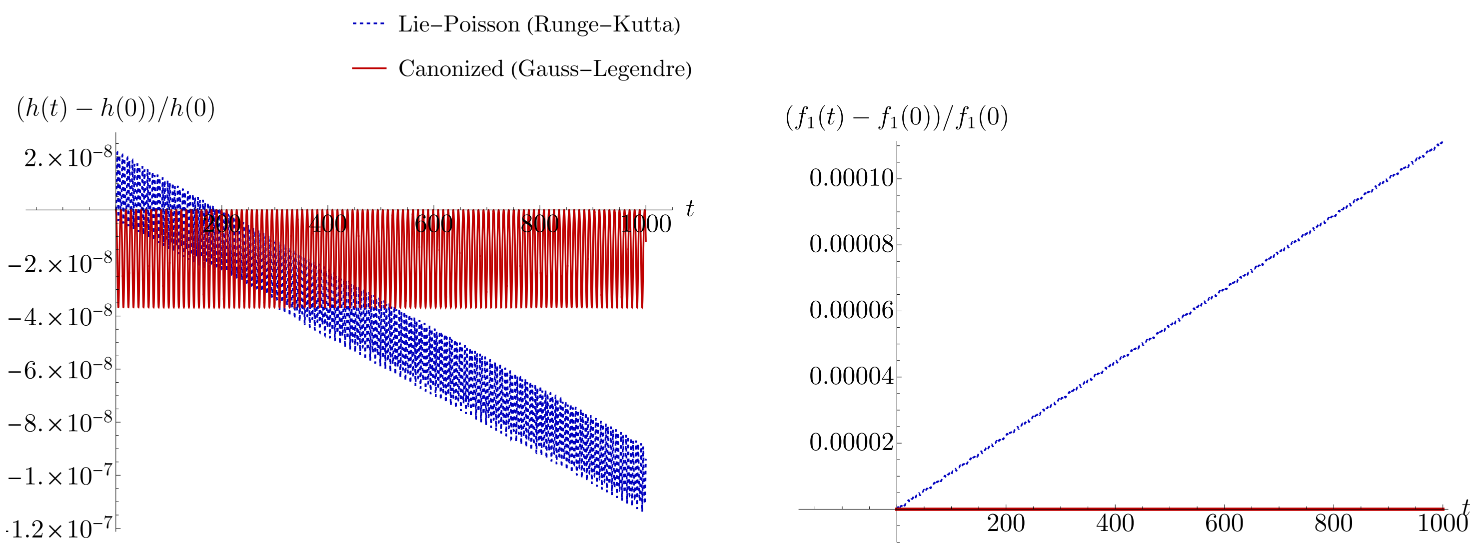



(a) Time evolution

(b) Lie–Poisson dynamics and invariants

FIGURE 1. (a) Time evolution of $\mu$ computed using the canonized system (25). The solutions are shown for the time interval $0 \le t \le 100$ with time step $\Delta t = 0.1$. (b) The red curve is the Lie–Poisson dynamics of the Kida vortex in $\mathfrak{g}^* = \mathfrak{so}(2,1)^* \cong \mathbb{R}^3$ computed using the canonized system (25) and mapped by $\mathbf{M}^+$ in (24). The green and orange surfaces are the level sets of the Hamiltonian $h$ and the Casimir $f_1$ from (22) and (19), respectively.

# Example: Kida Vortex (cont)




(a) Hamiltonian $h$ from (22) (b) Casimir $f_1$ from (19)

FIGURE 2. Time evolutions of relative errors in Hamiltonian $h$ and Casimir $f_1$ from the Kida system. The dashed blue curve is the $4^{\text{th}}$ order explicit Runge–Kutta method directly applied to Lie–Poisson equation (23) whereas the solid red curve is the $4^{\text{th}}$ order Gauss–Legendre method applied to the canonized system (25). The solutions are shown for the time interval $0 \leq t \leq 1000$ with time step $\Delta t = 0.1$. Note that, in (b), the red line is made thicker to make it visible; the actual variation is so small that it is barely visible if plotted with the same thickness as the blue line or as in (a).

# II. Simulated Annealinng

# Simulated Annealing

Use various bracket dynamics to effect extremization.

Many relaxation methods exist: gradient descent, etc.

Simulated annealing: an **artificial** dynamics that solves a variational principle with constraints **for equilibria states.**

# Double Bracket Simulated Annealing

Good Idea:

Vallis, Carnevale, and Young, Shepherd (1989)

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, H\} + ((\mathcal{F}, H)) = ((\mathcal{F}, \mathcal{F})) \geq 0$$

where

$$((F, G)) = \int d^3x \, \frac{\delta F}{\delta \chi} \mathcal{J}^2 \frac{\delta G}{\delta \chi}$$

Lyapunov function, $\mathcal{F}$, yields asymptotic stability to rearranged equilibrium.

• Maximizing energy at fixed Casimir: Works fine sometimes, but limited to circular vortex states ....

# Simulated Annealing (SA) with Generalized (Noncanonical) Dirac Brackets

Dirac Bracket:

$$\{F,G\}_D = \{F,G\} + \frac{\{F,C_1\}\{C_2,G\}}{\{C_1,C_2\}} - \frac{\{F,C_2\}\{C_1,G\}}{\{C_1,C_2\}}$$

Preserves any two incipient constraints $C_1$ and $C_2$.

New Idea:

Do simulated Annealing with Generalized Dirac Bracket

$$((F,G))_D = \int d\mathbf{x} \int d\mathbf{x}' \, \{F,\zeta(\mathbf{x})\}_D \; \mathcal{G}(\mathbf{x},\mathbf{x}') \; \{\zeta(\mathbf{x}'),G\}_D$$

Preserves any Casimirs of $\{F,G\}$ and Dirac constraints $C_{1,2}$

For successful implementation with contour dynamics see PJM (with Flierl) Phys. Plasmas **12** 058102 (2005).

# Double Bracket SA for Reduced MHD

M. Furukawa, T. Watanabe, pjm, and K. Ichiguchi, *Calculation of Large-Aspect-Ratio Tokamak and Toroidally-Averaged Stellarator Equilibria of High-Beta Reduced Magnetohydrodynamics via Simulated Annealing*, Phys. Plasmas **25**, 082506 (2018).

High-beta reduced MHD (Strauss, 1977) given by

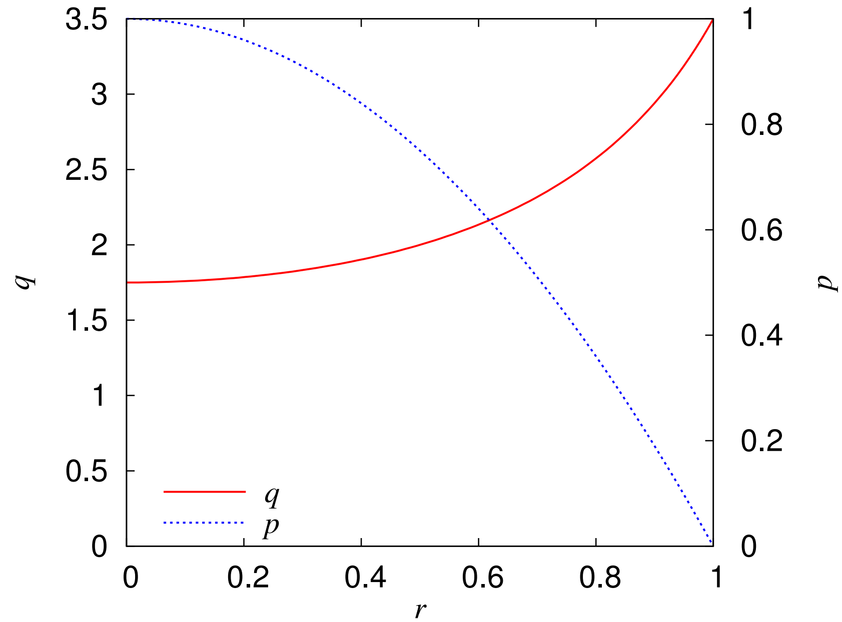
$$\frac{\partial U}{\partial t} = [U,\varphi] + [\psi, J] - \epsilon\frac{\partial J}{\partial \zeta} + [P,h]$$
$$\frac{\partial \psi}{\partial t} = [\psi,\varphi] - \epsilon\frac{\partial \varphi}{\partial \zeta}$$
$$\frac{\partial P}{\partial t} = [P,\varphi]$$

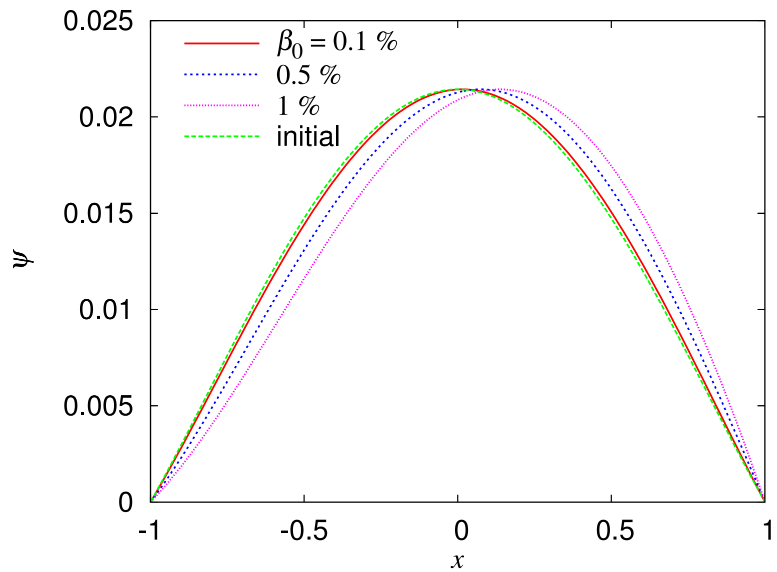
Extremization

$$\mathcal{F} = H + \sum_i C_i + \lambda^i P_i\,, \rightarrow \text{equilibria, maybe with flow}$$

$C$s Casimirs and $P$s dynamical invariants.

# Sample Double Bracket SA equilibria



# Double Bracket SA for Stability

M. Furukawa and pjm, *Stability analysis via simulated annealing and accelerated relaxation*, Phys. Plasmas **29, 102504 (2022).**

Since SA searches for an energy extremum, it can also be used for stability analysis when initiated from a state where a perturbation is added to an equilibrium. Three steps:

1) Choose **any** equilibrium of unknown stability.

2) Perturb the equilibrium with dynamically accessible (leaf) perturbation.

3) Perform double bracket SA.

If it finds the equilibrium, then is is an energy extremum and must be stable.

# Sample Double Bracket SA unstable equilibria

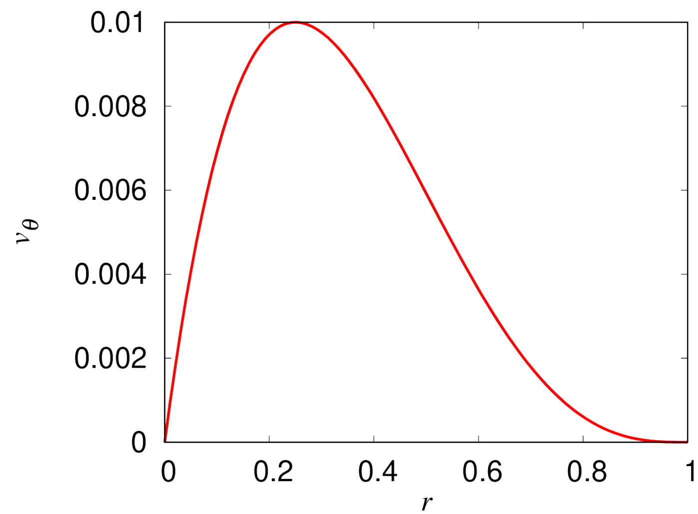
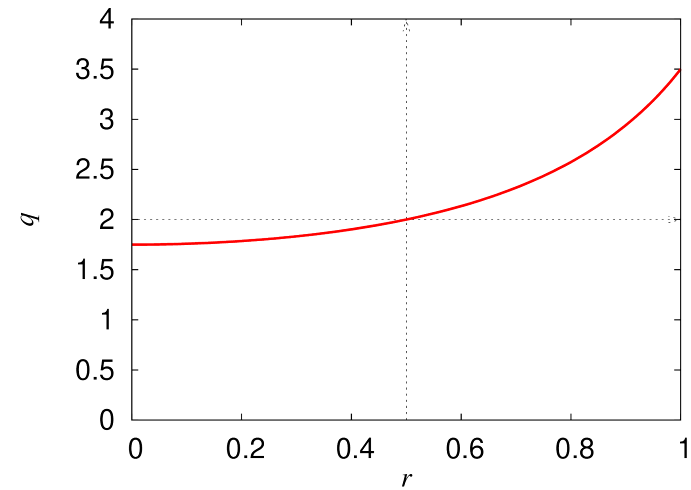
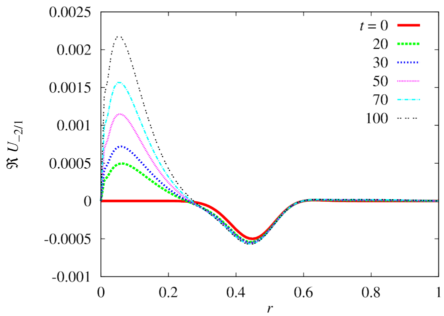
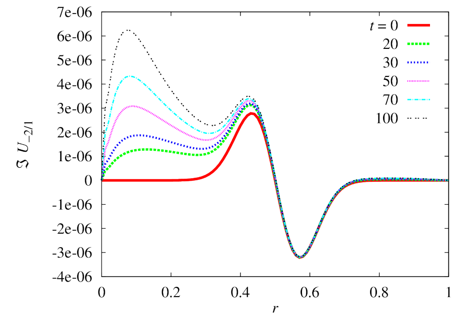



FIG. 12: Poloidal rotation velocity $v_\theta$ profile.

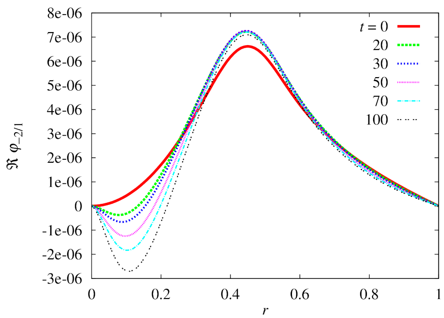




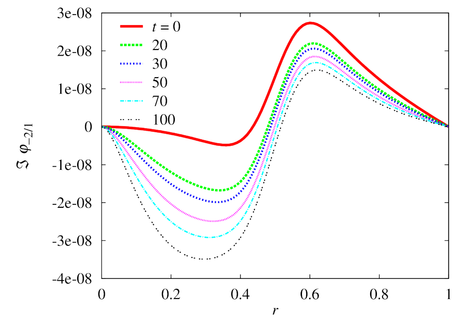

(a) Radial profile of $\Re U_{-2,1}$.



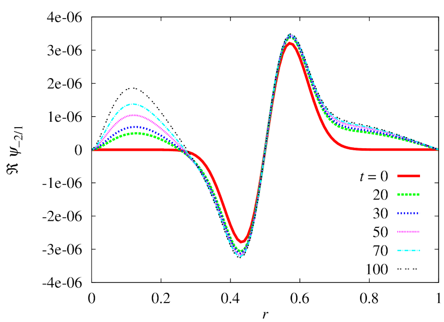

(b) Radial profile of $\Im U_{-2,1}$.



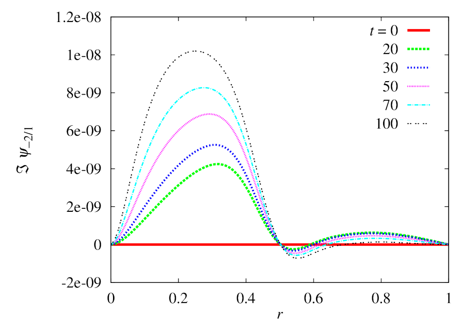

(c) Radial profile of $\Re \varphi_{-2,1}$.



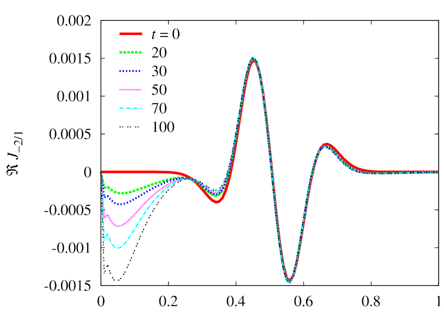

(d) Radial profile of $\Im \varphi_{-2,1}$.



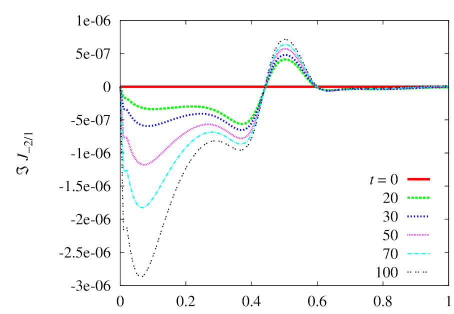

(e) Radial profile of $\Re \psi_{-2,1}$.




(f) Radial profile of $\Im \psi_{-2,1}$.




(g) Radial profile of $\Re J_{-2,1}$.




(h) Radial profile of $\Im J_{-2,1}$.

# III. Metriplectic Relaxation

# Metriplectic Dynamics – Entropy, Degeneracies, and 1st and 2nd Laws

- Casimirs of PB $\{\,,\,\}$ are 'candidate' entropies. Election of particular $S \in \{\text{Casimirs}\} \Rightarrow$ thermal equilibrium (relaxed) state.

- Generator: $\mathcal{F} = H + S$

- 1st Law: identify energy with Hamiltonian, $H$, then

$$\dot{H} = \{H, \mathcal{F}\} + (H, \mathcal{F}) = 0 + (H, H) + (H, S) = 0$$

  Foliate $\mathcal{Z}$ by level sets of $H$, with $(H, f) = 0 \; \forall \; f \in C^\infty(M)$.

- 2nd Law: entropy production

$$\dot{S} = \{S, \mathcal{F}\} + (S, \mathcal{F}) = (S, S) \geq 0$$

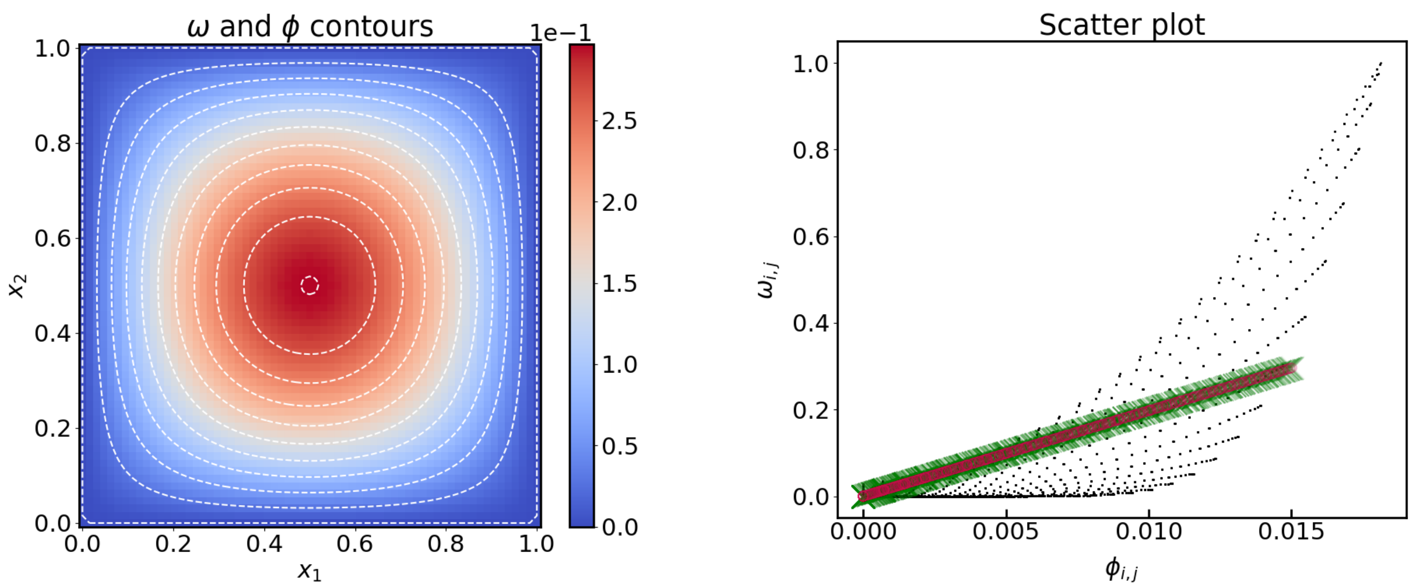
  Lyapunov relaxation to the equilibrium state: $\nabla\mathcal{F} = 0$.

## Metriplectic Simulated Annealing

Extremizes an entropy (Casimir) at fixed energy (Hamiltonian)

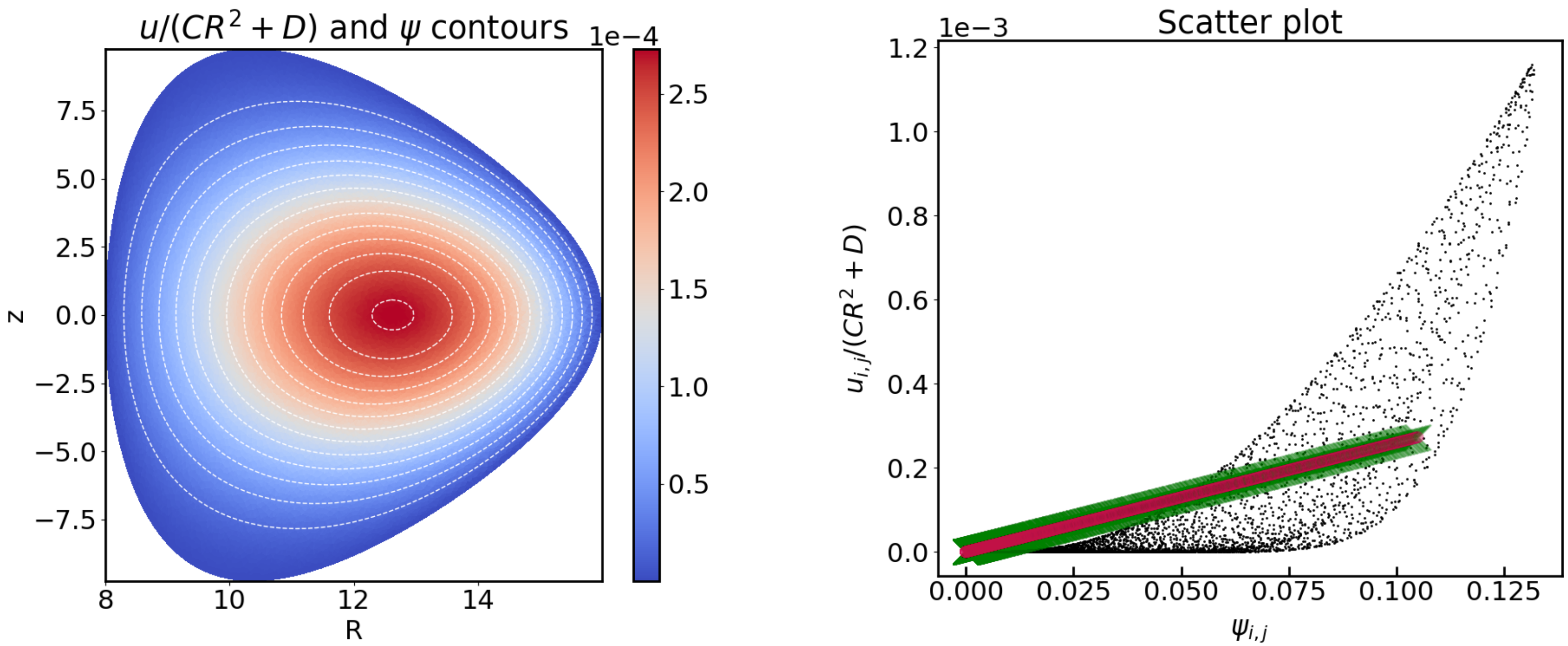
C. Bressen Ph.D. Thesis TUM, Garching 2023

Two cases: 2D Euler and Grad Shafranov MHD equilibria.




(a) **Color plot.** (b) **Scatter plot.**

Figure 6.7: **Relaxed state for the test case *euler-ilgr*.** The same as in Figure 6.2, but for the collision-like operator.




(a) **Color plot.**

(b) **Scatter plot.**

Figure 6.29: **Relaxed state for the *gs-imgc* test case.** The same as in Figure 6.23, but for the collision-like operator and the case of the Czarny domain discussed in Section A.4.2. With respect to Figure 6.27(b) for the diffusion-like operator, we see from (b) that the agreement between the relaxed state and the prediction of the variational principle is better.

## Summary

I. Family of Poisson Integrators

II. Simulated Annealing for Stability

III. Metriplectic Simulated Annealing