On Metriplectic Dynamics: Joint Hamiltonian and Dissipative Dynamics

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Overview: Structure and Numerics. A potpourri.

Codifying Dissipation – Some History

Is there a framework for dissipation akin to the Hamiltonian formulation for nondissipative systems?

Rayleigh (1873): $\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_\nu}\right) - \left(\frac{\partial \mathcal{L}}{\partial q_\nu}\right) + \left(\frac{\partial \mathcal{F}}{\partial \dot{q}_\nu}\right) = 0$

Linear dissipation e.g. of sound waves. *Theory of Sound*.

Cahn-Hilliard (1958): $\frac{\partial n}{\partial t} = \nabla^2 \frac{\delta F}{\delta n} = \nabla^2 \left(n^3 - n - \nabla^2 n\right)$

Phase separation, nonlinear diffusive dissipation, binary fluid ..

Other Gradient Flows: $\frac{\partial \psi}{\partial t} = \mathcal{G}\,\frac{\delta F}{\delta \psi}$

Otto, Ricci Flows, Poincarè conjecture on S^3, Perlman (2002)...

Poisson Brackets and Bracket Dissipation

Noncanonical Poisson Brackerts (pjm 1980)

Degenerate Antisymmetric Bracket (Kaufman and pjm 1982)

Double Brackets (Vallis, Carnevale; Brockett, Bloch ... 1990)

Metriplectic Dynamics (pjm 1984,1986)

Generic (Grmela, Oettinger 1997)

Poisson Brackets and Bracket Dissipation

Noncanonical Poisson Brackerts (pjm 1980s)

Degenerate Antisymmetric Bracket (Kaufman and pjm 1982)

$*$ Double Bracket (Vallis, Carnevale; Brockett, Bloch ... 1990)

$*$ Metriplectic Dynamics (pjm 1984,1986)

Noncanonical MHD (pjm & Greene 1980)

Equations of Motion:

$$
\begin{aligned}
\text{Force} \qquad \rho\frac{\partial \boldsymbol{v}}{\partial t} &= -\rho\boldsymbol{v}\cdot\nabla\boldsymbol{v} - \nabla p + \frac{1}{c}\boldsymbol{J}\times\boldsymbol{B} \\
\text{Density} \qquad \frac{\partial \rho}{\partial t} &= -\nabla\cdot(\rho\boldsymbol{v}) \\
\text{Entropy} \qquad \frac{\partial s}{\partial t} &= -\boldsymbol{v}\cdot\nabla s \\
\text{Ohm's Law} \qquad \boldsymbol{E} &+ \boldsymbol{v}\times\boldsymbol{B} = \eta\boldsymbol{J} = \eta\nabla\times\boldsymbol{B} \approx 0 \\
\text{Magnetic Field} \qquad \frac{\partial \boldsymbol{B}}{\partial t} &= -\nabla\times\boldsymbol{E} = \nabla\times(\boldsymbol{v}\times\boldsymbol{B})
\end{aligned}
$$

Energy:

$$
H = \int_D d^3x \left(\frac{1}{2}\rho|\boldsymbol{v}|^2 + \rho U(\rho, s) + \frac{1}{2}|\boldsymbol{B}|^2\right)
$$

Thermodynamics:

$$
p = \rho^2\frac{\partial U}{\partial \rho} \qquad\qquad T = \frac{\partial U}{\partial s} \qquad \text{or} \qquad p = \kappa\rho^\gamma
$$

Noncanonical Bracket:

$$
\begin{aligned}
\{F,G\} \;=\; -\int_D d^3x \Bigg(& \left[\frac{\delta F}{\delta \rho}\nabla\frac{\delta G}{\delta \boldsymbol{v}} - \frac{\delta G}{\delta \rho}\nabla\frac{\delta F}{\delta \boldsymbol{v}}\right] + \left[\frac{\delta F}{\delta \boldsymbol{v}} \cdot \left(\frac{\nabla\times\boldsymbol{v}}{\rho} \times \frac{\delta F}{\delta \boldsymbol{v}}\right)\right] \\
& + \frac{\nabla s}{\rho} \cdot \left[\frac{\delta F}{\delta \boldsymbol{v}} \cdot \nabla\frac{\delta G}{\delta s} - \frac{\delta G}{\delta \boldsymbol{v}} \cdot \nabla\frac{\delta F}{\delta s}\right] \\
& + \boldsymbol{B} \cdot \left[\frac{1}{\rho}\frac{\delta F}{\delta \boldsymbol{v}} \cdot \nabla\frac{\delta G}{\delta \boldsymbol{B}} - \frac{1}{\rho}\frac{\delta G}{\delta \boldsymbol{v}} \cdot \nabla\frac{\delta F}{\delta \boldsymbol{B}}\right] \\
& + \boldsymbol{B} \cdot \left[\nabla\left(\frac{1}{\rho}\frac{\delta F}{\delta \boldsymbol{v}}\right) \cdot \frac{\delta G}{\delta \boldsymbol{B}} - \nabla\left(\frac{1}{\rho}\frac{\delta G}{\delta \boldsymbol{v}}\right) \cdot \frac{\delta F}{\delta \boldsymbol{B}}\right]\Bigg) .
\end{aligned}
$$

Dynamics:

$$
\frac{\partial \rho}{\partial t} = \{\rho, H\}\,, \quad \frac{\partial s}{\partial t} = \{s, H\}\,, \quad \frac{\partial \boldsymbol{v}}{\partial t} = \{\boldsymbol{v}, H\}\,, \text{ and } \frac{\partial \boldsymbol{B}}{\partial t} = \{\boldsymbol{B}, H\}\,.
$$

Densities:

$$
\boldsymbol{M} := \rho\boldsymbol{v} \qquad \sigma := \rho s \qquad \text{Lie – Poisson form}
$$

Casimir Invariants

Casimir Invariants:

$$\{F, C\}^{MHD} = 0 \qquad \forall \text{ functionals } F.$$

Casimirs Invariant entropies:

$$C_S = \int d^3x\, \rho f(s)\,, \qquad \text{f arbitrary}$$

Casimirs Invariant helicities:

$$C_B = \int d^3x\, \boldsymbol{B} \cdot \boldsymbol{A}\,, \qquad C_V = \int d^3x\, \boldsymbol{B} \cdot \boldsymbol{v}$$

Helicities have topological content, linking etc.

Hamilton's Equations

Phase Space with Canonical Coordinates: (q, p)

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

Equations of Motion:

$$\boxed{\dot{p}_i = -\frac{\partial H}{\partial q^i}\,, \qquad \dot{q}^i = \frac{\partial H}{\partial p_i}\,,} \qquad i = 1, 2, \ldots N$$

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

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

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

Noncanonical Hamiltonian Structure

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

Noncanonical Coordinates:

$$\dot{z}^\alpha = \{z^\alpha, H\} = J^{\alpha\beta}(z)\frac{\partial H}{\partial z^\beta}$$

Noncanonical Poisson Bracket:

$$\{A, B\} = \frac{\partial A}{\partial z^\alpha} J^{\alpha\beta}(z) \frac{\partial B}{\partial z^\beta}$$

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: $det J \neq 0 \Longrightarrow J \rightarrow J_c$ Canonical Coordinates

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

Flow on Poisson Manifold

Definition. A Poisson manifold $\mathcal{Z}$ is differentiable manifold with bracket

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

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

i) bilinear,
ii) antisymmetric,
iii) Jacobi, and
iv) Leibniz, i.e., acts as a derivation.

Flows are integral curves of noncanonical Hamiltonian vector fields, JdH.

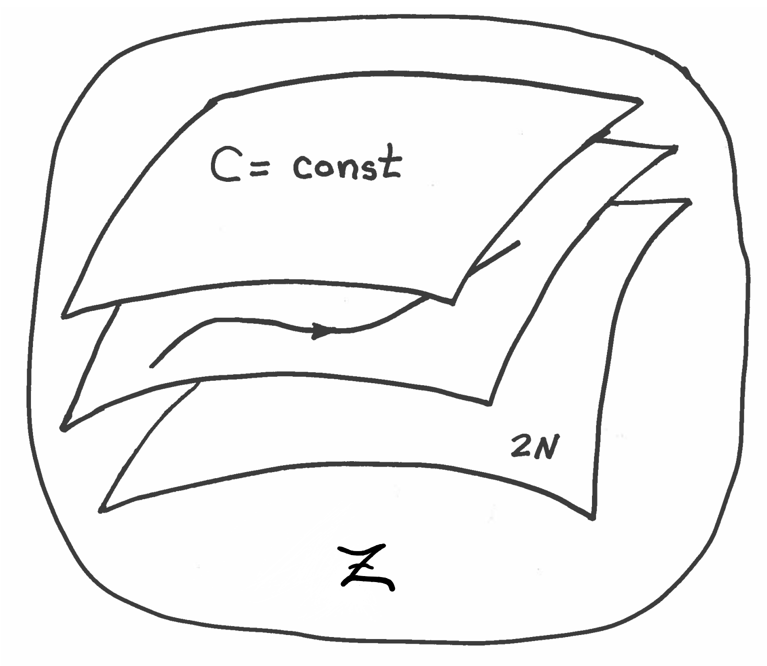
Because of degeneracy, $\exists$ functions C st $\{A, C\} = 0$ for all $A \in C^\infty(\mathcal{Z})$. Called Casimir invariants (Lie's distinguished functions!).

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

Degeneracy in $J \Rightarrow$ Casimirs:

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

Lie-Darboux Foliation by Casimir (symplectic) leaves:



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 $f, g \in C^\infty(\mathfrak{g}^*)$ and $z \in \mathfrak{g}^*$.

Lie-Poisson bracket has the form

$$
\begin{aligned}
\{f, g\} &= \langle z, [\nabla f, \nabla g] \rangle \\
&= \frac{\partial f}{\partial z^i} c^{ij}{}_k \, z_k \frac{\partial g}{\partial z^j} \,, \qquad\qquad i, j, k = 1, 2, \ldots, \dim \mathfrak{g}
\end{aligned}
$$

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

Poisson Integration

Symplectic integrators (1980s): time step with canonical transformation.

Poisson integrators (timely): time step with canonical transformation.

Symplectic on leaf but remain 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).

Canonization of Lie-Poisson Brackets

Vlasov Lie-Poisson Bracket:

$$\{F,G\} = \int d^3x d^3v\, f(x,v)\, \left[\frac{\delta F}{\delta f}, \frac{\delta G}{\delta f}\right]$$

* Clebsch potentials, making a bigger system, $f = [\chi, \psi]$, works also for QM with Wigner-Weyl by replacing [,] by Moyal bracket (Bialynicki-Birula & pjm 1991). Nonlinearity via Hamiltonian.

* Mean field (self-consistent) Hamiltonian-Jacobi theory of Vlasov in terms of mixed variable generating function $S(q,P,t)$ with Van Vleck determinant (Pfirsch, pjm 1985,2012). Related to QM?

* Lie generators on a symplectic leaf. Ye et al. (1991).

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 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

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

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

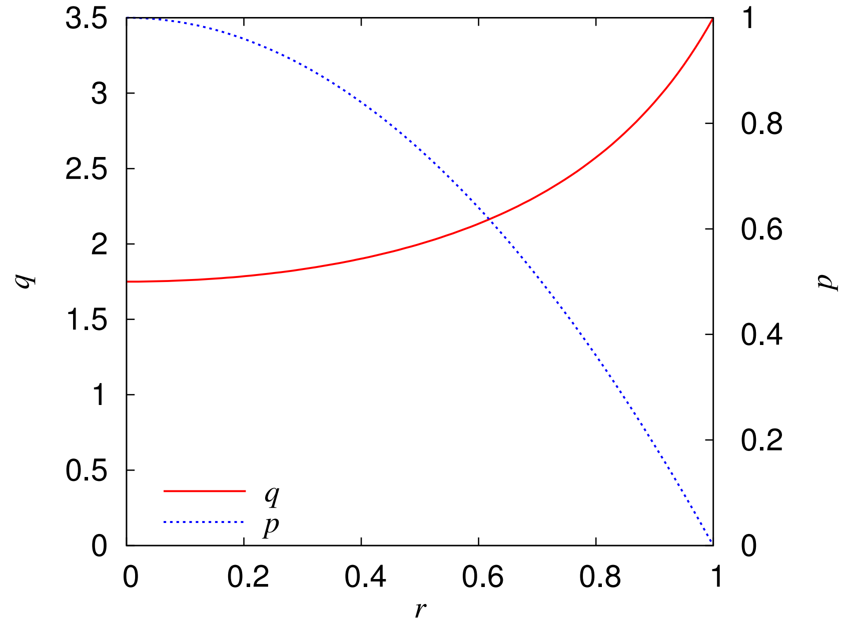
$$\begin{aligned}
\frac{\partial U}{\partial t} &= [U, \varphi] + [\psi, J] - \epsilon \frac{\partial J}{\partial \zeta} + [P, h] \\
\frac{\partial \psi}{\partial t} &= [\psi, \varphi] - \epsilon \frac{\partial \varphi}{\partial \zeta} \\
\frac{\partial P}{\partial t} &= [P, \varphi]
\end{aligned}$$

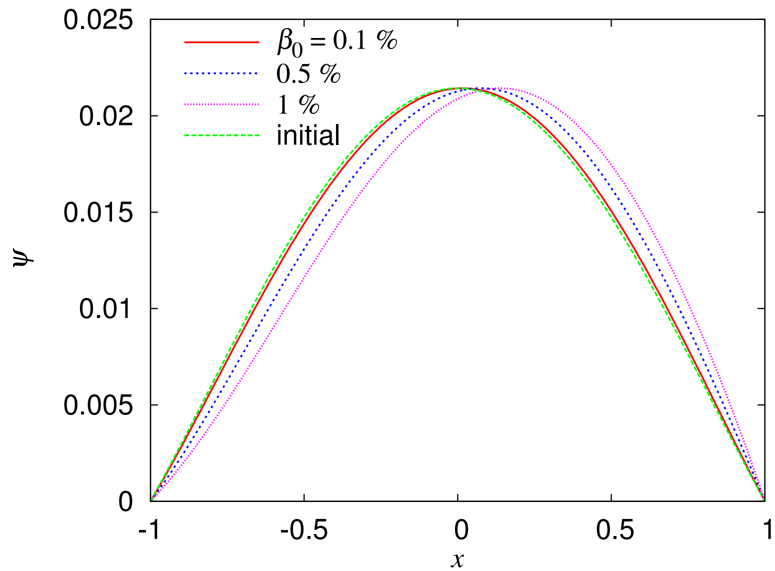
Extremization

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

Cs Casimirs and Ps dynamical invariants.

Sample Double Bracket SA equilibria





Nested Tori are level sets of ψ; q gives pitch of helical $\boldsymbol{B}$-lines.

Double Bracket SA for Stability

M. Furukawa and P. J. Morrison, *Stability analysis via simulated annealing and accelerated relaxation* , Phys. Plasmas, 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

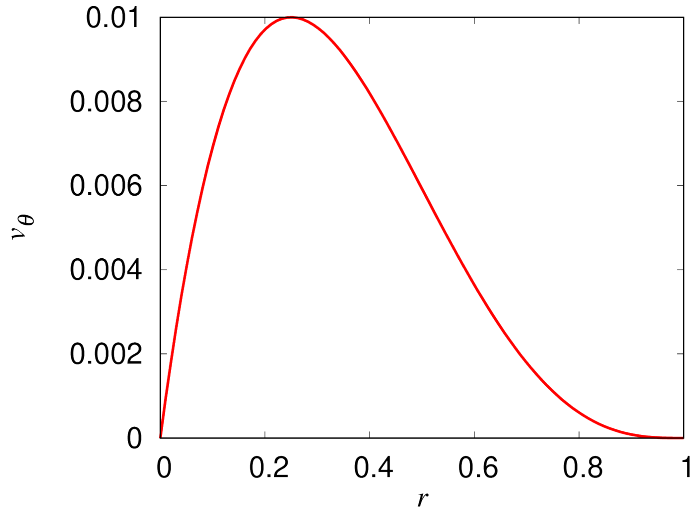
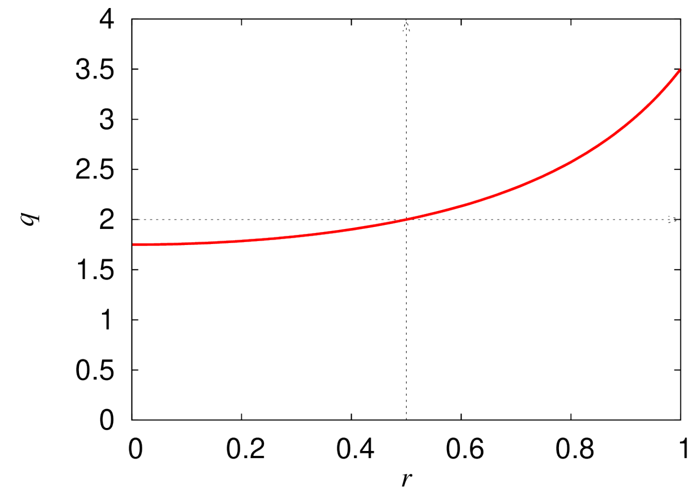
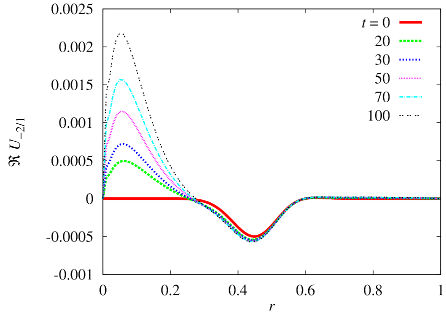
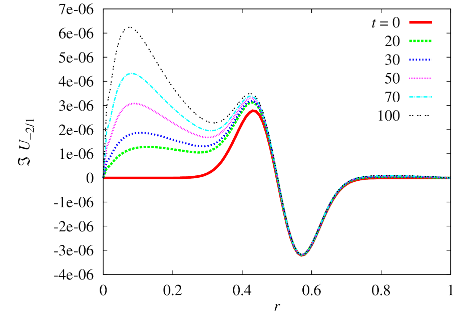


FIG. 12: Poloidal rotation velocity v_θ profile.

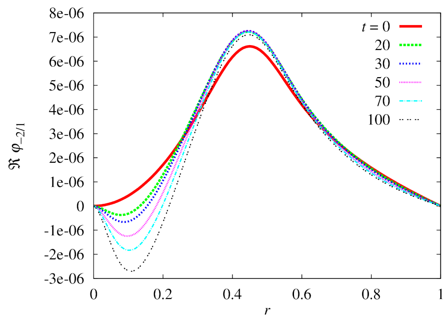




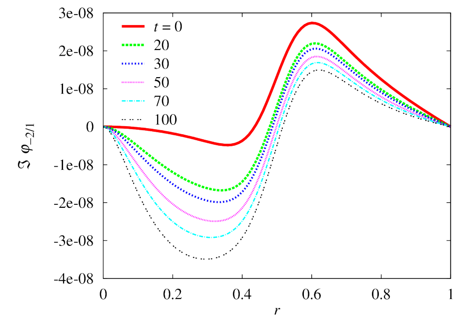
(a) Radial profile of $\Re\, U_{-2,1}$.



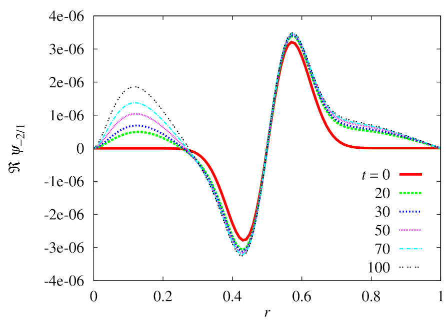
(b) Radial profile of $\Im\, U_{-2,1}$.



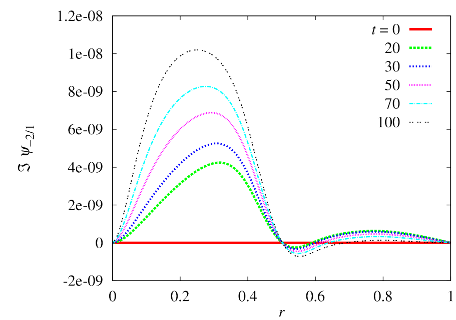
(c) Radial profile of $\Re\, \varphi_{-2,1}$.



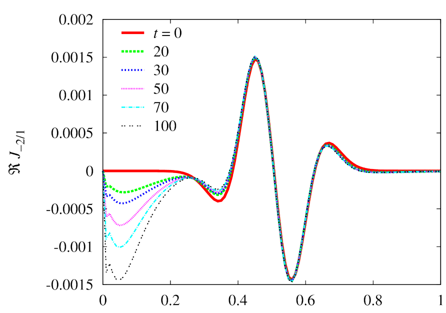
(d) Radial profile of $\Im\, \varphi_{-2,1}$.



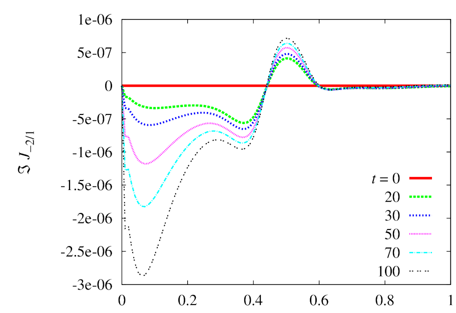
(e) Radial profile of $\Re\, \psi_{-2,1}$.



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



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



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

Metriplectic Dynamics

A dynamical model of thermodynamics that ‘captures’:.

- First Law: conservation of energy

- Second Law: entropy production

Entropy, Degeneracies, and 1st and 2nd Laws

- Casimirs of $[,]$ 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

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

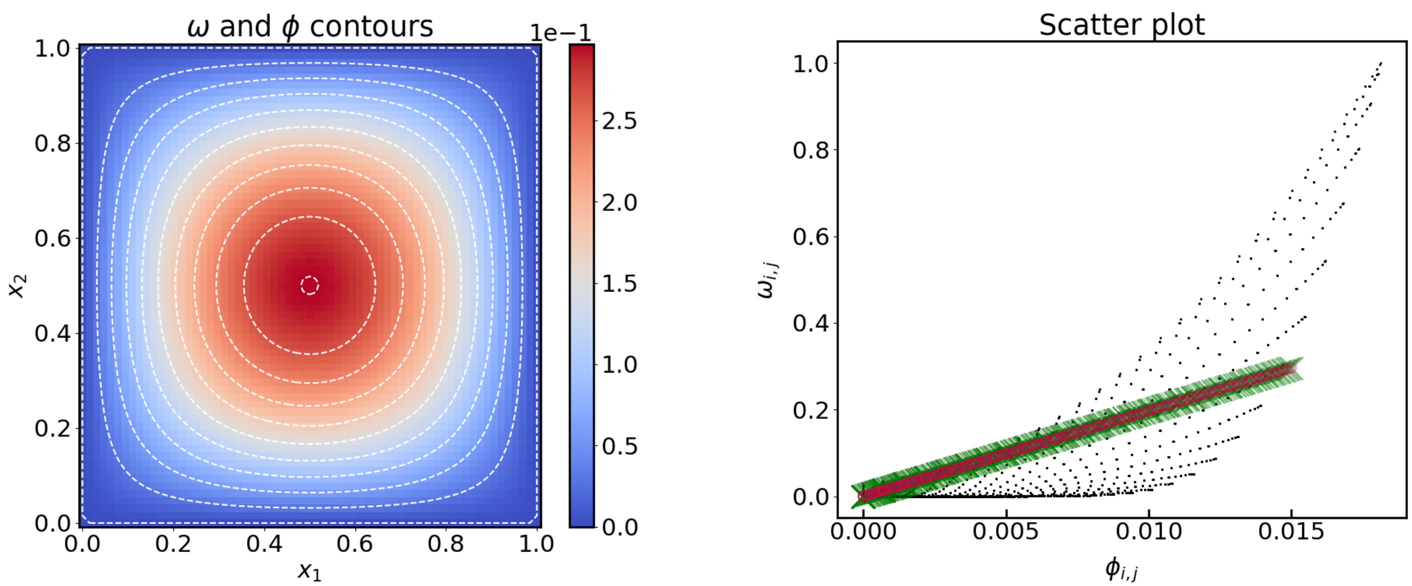
  Lyapunov relaxation to the equilbrium state: $\nabla \mathcal{F} = 0$.

Metriplectic Simulated Annealing

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

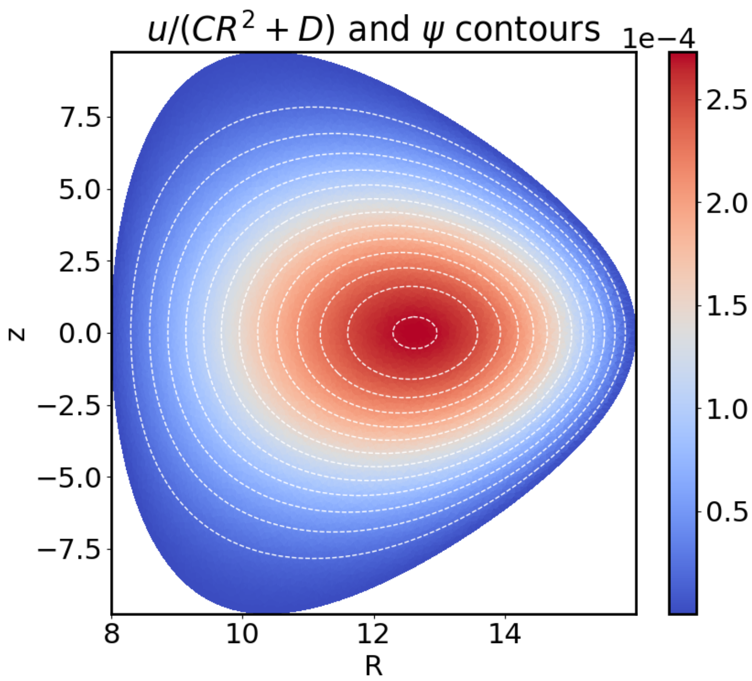
C. Bressen Ph.D. Thesis TUM, Garching 2022

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

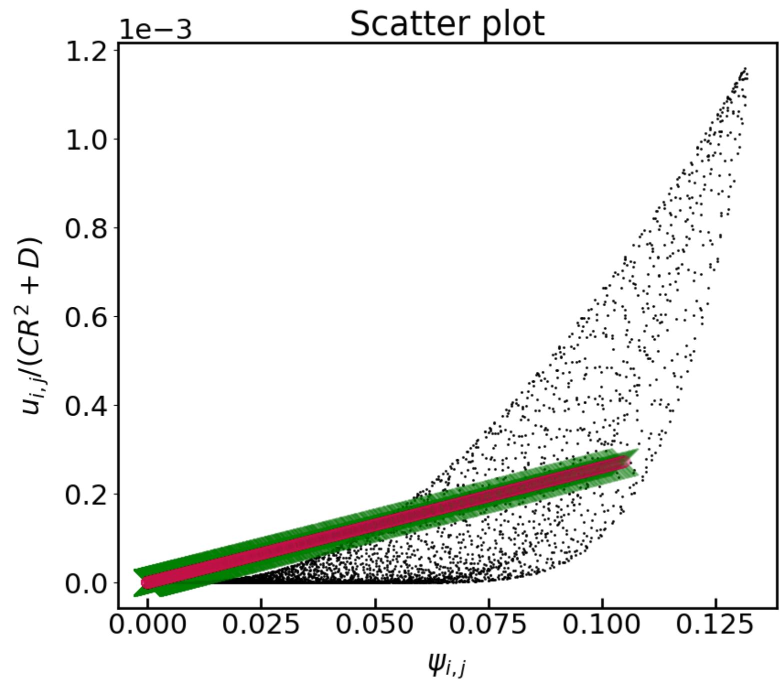


(a) **Color plot.** (b) **Scatter plot.**

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.