The General Metriplectic Formalism for Describing Dissipation and its Computational Uses

Philip J. Morrison

Department of Physics and Institute for Fusion Studies The University of Texas at Austin morrison@physics.utexas.edu http://www.ph.utexas.edu/~morrison/

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Collaborators: G. Flierl, M. Furukawa, C. Bressan, O. Maj, M. Kraus, E. Sonnendruecker, ...

Codifying Dissipation – Some History

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

<u>Rayleigh</u> (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*.

<u>Cahn-Hilliard</u>: (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 ...

<u>Other</u> 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 1980s)

Degenerate Antisymmetric Bracket (Kaufman and pjm, 1982)

Double Brackets (Vallis, Carnevale, Bloch, ... 1989)

Metriplectic Dynamics (pjm 1984,1986)

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- * Double Brackets (Vallis, Carnevale, Bloch, ... 1989)
- * Metriplectic Dynamics (pjm 1984,1986)

Noncanonical MHD (pjm & Greene 1980)

Equations of Motion:

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

Energy:

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

Thermodynamics:

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

Noncanonical Bracket:

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

Dynamics:

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

Casimir Invariants

Casimir Invariants:

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

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: $H(q, p) \leftarrow \text{the energy}$

Equations of Motion:

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

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

$$\dot{z}^{\alpha} = J_{c}^{\alpha\beta} \frac{\partial H}{\partial z^{\beta}} = \{ z^{\alpha}, H \}_{c}, \qquad (J_{c}^{\alpha\beta}) = \begin{pmatrix} 0_{N} & I_{N} \\ -I_{N} & 0_{N} \end{pmatrix},$$

 $J_c := \underline{Poisson tensor}$, Hamiltonian bi-vector, cosymplectic form

Noncanonical Hamiltonian Structure

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:

$$\{A,B\} = \frac{\partial A}{\partial z^a} J^{ab}(z) \frac{\partial B}{\partial z^b}$$

Poisson Bracket Properties:

 $\begin{array}{ll} \text{antisymmetry} & \longrightarrow & \{A, B\} = -\{B, A\} \\ \text{Jacobi identity} & \longrightarrow & \{A, \{B, C\}\} + \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0 \\ \text{Leibniz} & \longrightarrow & \{AC, B\} = A\{C, B\} + \{C, B\}A \end{array}$

G. Darboux: $det J \neq 0 \implies J \rightarrow J_c$ Canonical Coordinates

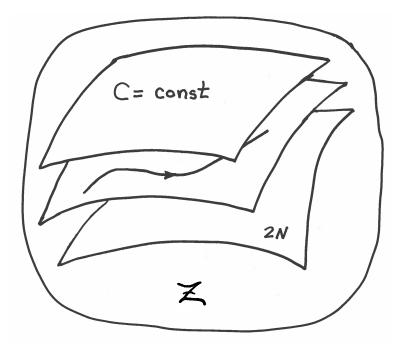
Sophus Lie: $detJ = 0 \implies$ Canonical Coordinates plus <u>Casimirs</u> (Lie's distinguished functions!)

Poisson (phase space) Manifold 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 (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).

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)

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

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.

• <u>Maximizing</u> 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 Stel-larator Equilibria of High-Beta Reduced Magnetohydrodynamics via Simulated Annealing*, Phys. Plasmas **25**, 082506 (2018).

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

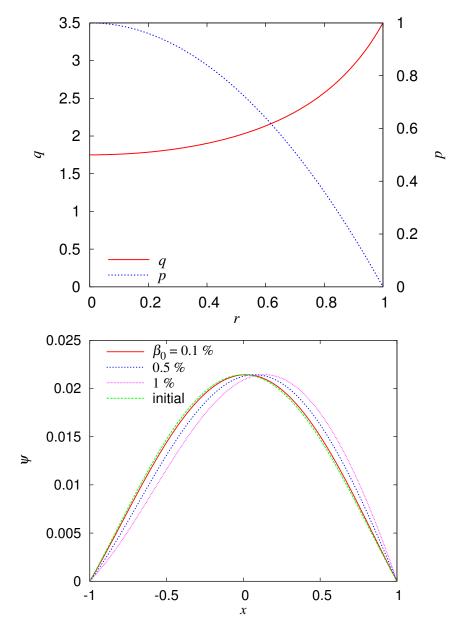
$$\frac{\partial U}{\partial t} = [U, \varphi] + [\psi, J] - \epsilon \frac{\partial J}{\partial \zeta} + [P, h]$$
$$\frac{\partial \psi}{\partial t} = [\psi, \varphi] - \epsilon \frac{\partial \varphi}{\partial \zeta}$$
$$\frac{\partial P}{\partial t} = [P, \varphi]$$

Extremization

$$\mathcal{F} = H + \sum_{i} C_{i} + \lambda^{i} P_{i}, \rightarrow \text{equilibria}, \text{ maybe with flow}$$

Cs Casimirs and Ps dynamical invariants.

Sample Double Bracket SA equilibria



Double Bracket SA for Stability

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

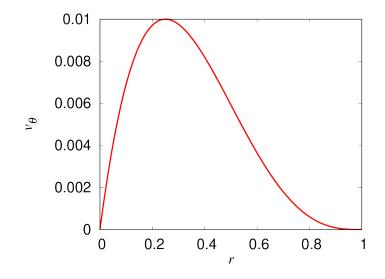
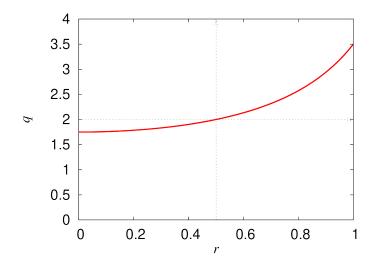
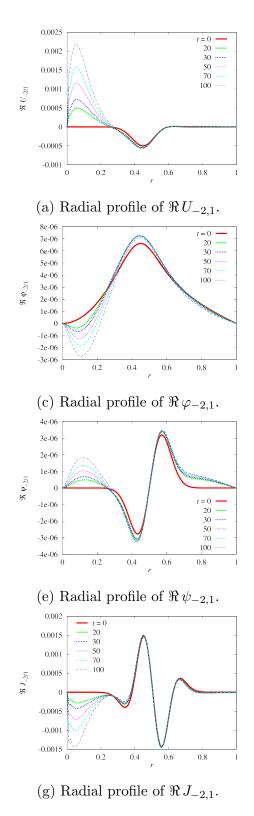
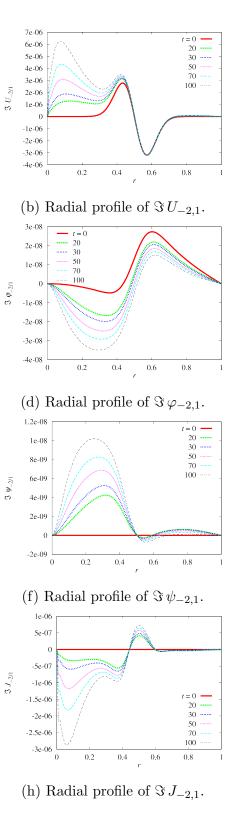


FIG. 12: Poloidal rotation velocity v_{θ} profile.







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
 H
 = [H, F] + (H, F) = 0 + (H, H) + (H, S) = 0
 Foliate Z by level sets of H, with (H, f) = 0 ∀ f ∈ C[∞](M).
- 2nd Law: entropy production

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

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.

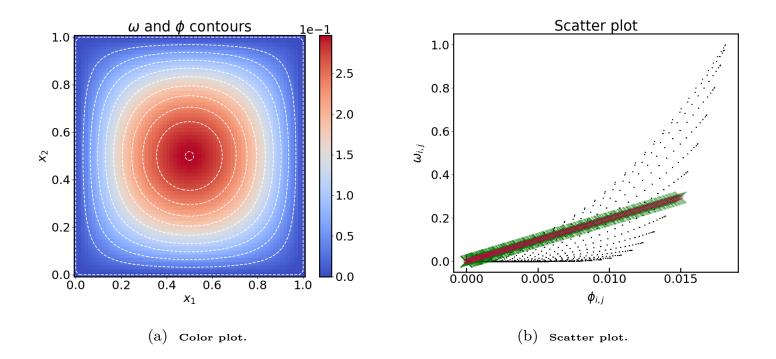


Figure 6.7: Relaxed state for the test case *euler-ilgr*. The same as in Figure 6.2, but for the collision-like operator.

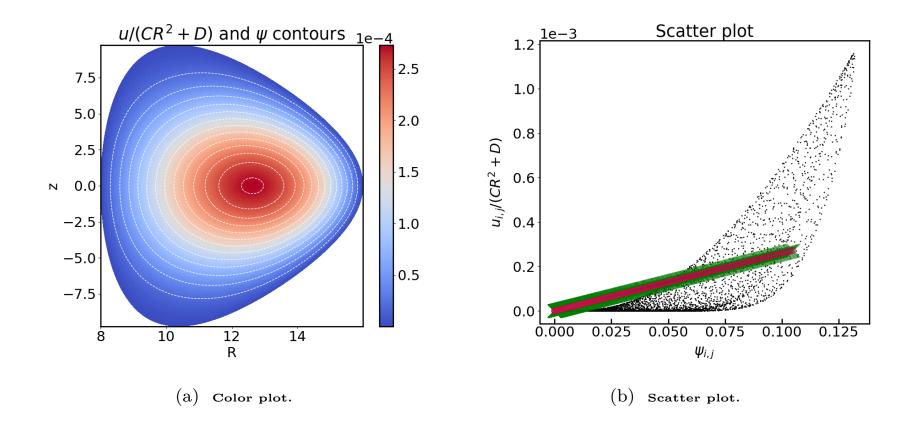


Figure 6.29: Relaxed state for the *gs-imgc* test case. The same as in Figure 6.23, but for the collision-like operator and the case of the Czarny domain discussed in Section A.4.2. With respect to Figure 6.27(b) for the diffusion-like operator, we see from (b) that the agreement between the relaxed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