

On an inclusive curvature-like framework for describing dissipation: metriplectic 4-bracket dynamics

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Geometry of metriplectic 4-brackets: with Michael Updike

pjm & M. Updike, arXiv:2306.06787v2 [math-ph]

→ **Theory of thermodynamically consistent theories!**

Thermodynamic Consistency – Examples

Navier-Stokes (**inconsistent**):

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

$$H = \int_{\Omega} \rho_0 |\mathbf{v}|^2 / 2 \quad \text{and} \quad \dot{H} \leq 0$$

Thermodynamic Navier-Stokes (**consistent**) (Eckart 1940):

$$\partial_t \mathbf{v} = -\mathbf{v} \cdot \nabla \mathbf{v} - \frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot \mathcal{T} \quad \leftarrow \quad \mathcal{T} \text{ viscous stress tensor}$$

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

$$\partial_t s = -\mathbf{v} \cdot \nabla s - \frac{1}{\rho T} \nabla \cdot \mathbf{q} + \frac{1}{\rho T} \mathcal{T} : \nabla \mathbf{v}, \quad \mathbf{q} = -\kappa \nabla T \quad \leftarrow \quad \mathcal{T} \text{ heat flux}$$

$$H = \int_{\Omega} \rho |\mathbf{v}|^2 / 2 + \rho U(\rho, s), \quad \dot{H} = 0 \quad \text{and} \quad \dot{S} = \int_{\Omega} \rho s$$

Theories & Models \rightarrow Dynamics

Goal:

Predict the future or explain the past \Rightarrow

$$\dot{z} = V(z), \quad z \in \mathcal{Z}, \text{ Phase Space}$$

Ultimately a dynamical system. Vector fields on manifold.

Maps, ODEs, PDEs, etc.

Whence vector field V ?

- Fundamental parent theory (microscopic, N interacting gravitating or charged particles, BBGKY hierarchy, Vlasov-Maxwell system, ...). Identify small parameters, rigorous asymptotics

\rightarrow

Reduced Computable Model V .

- Phenomena based modeling using known properties, constraints, etc. used to intuit \rightarrow

Reduced Computable Model V . \leftarrow structure can be useful.

Types of Vector Fields, $V(z)$ (cont)

Only (?) Natural Split:

$$V(z) = V_H + V_D$$

- Hamiltonian vector fields, V_H : conservative, properties, etc.
- Dissipative vector fields, V_D : not conservative of something, relaxation/asymptotic stability, etc.

General Hamiltonian Form:

$$\text{finite dim} \rightarrow V_H = J \frac{\partial H}{\partial z} \quad \text{or} \quad V_H = \mathcal{J} \frac{\delta H}{\delta \psi} \quad \leftarrow \infty \text{ dim}$$

where $J(z)$ is Poisson tensor/operator and H is the Hamiltonian. Basic product decomposition.

General Dissipation:

$$V_D = ? \dots \quad \rightarrow \quad V_D = G \frac{\partial F}{\partial z}$$

Why investigate? General properties of theory. Build in thermodynamic consistency. Geometry? Useful for computation.

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*.

Gay-Balmaz & Yoshimura (2017) (C. Eldred, 2020):

Lagrangian variational formulation with constraints.

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

Phase separation, nonlinear diffusive dissipation, binary fluid ..

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

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

Metriplectic Dynamics

(Metric \cup Symplectic Flows)

- Formalism for natural split of vector fields
- 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 theory:** “curvature” as dissipation

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

Hamiltonian Review

Poisson Bracket: $\{f, g\}$

Hamilton's Canonical Equations

Phase Space with Canonical Coordinates: (q, p)

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

Equations of Motion:

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

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

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

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

Noncanonical Hamiltonian Structure

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

Noncanonical Coordinates:

$$\dot{z}^i = \{z^i, H\} = J^{ij}(z) \frac{\partial H}{\partial z^j}$$

Noncanonical Poisson Bracket:

$$\{f, g\} = \frac{\partial f}{\partial z^i} J^{ij}(z) \frac{\partial g}{\partial z^j}$$

Poisson Bracket Properties:

antisymmetry $\longrightarrow \{f, g\} = -\{g, f\}$

Jacobi identity $\longrightarrow \{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$

Leibniz $\longrightarrow \{fh, g\} = f\{h, g\} + \{h, g\}f$

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

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

Poisson Brackets – Flows on Poisson Manifolds

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

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

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

- bilinear,
- antisymmetric,
- Jacobi, and
- Leibniz, i.e., acts as a derivation \Rightarrow vector field.

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

$$\{f, g\} = \langle df, Jdg \rangle = J(df, dg).$$

J the Poisson tensor/operator. Flows are integral curves of noncanonical Hamiltonian vector fields, JdH , i.e.,

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

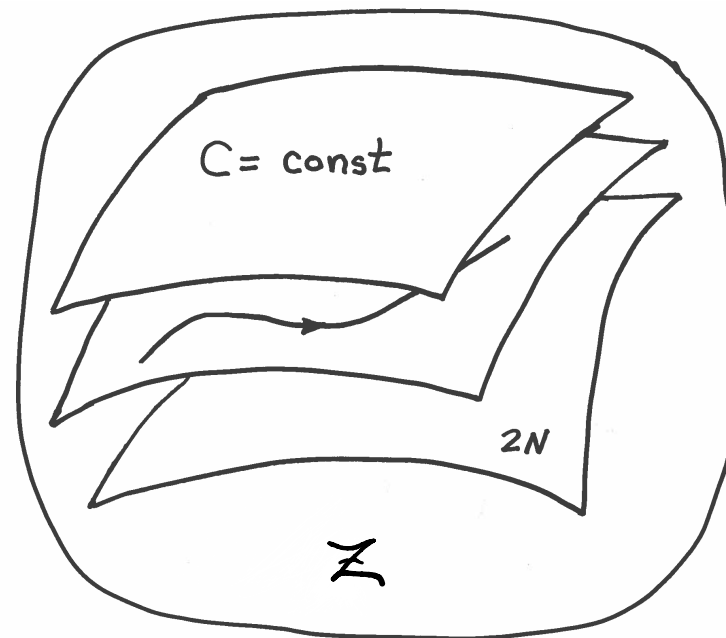
Because of degeneracy, \exists functions C st $\{f, C\} = 0$ for all $f \in C^\infty(\mathcal{Z})$. Casimir invariants (Lie's distinguished functions!).

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

Degeneracy in $J \Rightarrow$ Casimirs:

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

Lie-Darboux Foliation by Casimir (symplectic) leaves:



Metriplectic 4-Bracket: $(f, k; g, n)$

Why a 4-Bracket?

- Two slots for two fundamental functions: Hamiltonian, H , and Entropy (Casimir), S .
- There remains two slots for bilinear bracket: one for observable one for generator (\mathcal{F} ?) s.t. $\dot{H} = 0$ and $\dot{S} \geq 0$.
- 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):

$$(\cdot, \cdot; \cdot, \cdot): \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \rightarrow \Lambda^0(\mathcal{Z})$$

For functions $f, k, g, n \in \Lambda^0(\mathcal{Z})$

$$(f, k; g, n) := R(df, dk, dg, dn),$$

In a coordinate patch the metriplectic 4-bracket has the form:

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

- A blend of my previous ideas: Two important functions H and S , symmetries, curvature idea, multilinear brackets.
- Manifolds with both Poisson tensor, J^{ij} , and compatible quadravector R^{ijkl} , where S and H come from Hamiltonian part.

Metriplectic 4-Bracket Properties

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

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

(ii) algebraic identities/symmetries

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

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

$$(f, k; g, n) = (g, n; f, k)$$

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

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

which is manifest in coordinates. Here, as usual, fh denotes pointwise multiplication. Symmetries of algebraic curvature without cyclic identity. Often see R^l_{ijk} or R_{lijk} but not R^{lijk} !

Minimal Metriplectic if above and

(iv) positive semidefiniteness

$$(f, g; f, g) \geq 0$$

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

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

$$(f, k; g, n) = (g, n; f, k)$$

$$(f, k; g, n) + (f, g; n, k) + (f, n; k, g) = 0 \quad \leftarrow \text{not needed}$$

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1980s Binary 2-Brackets and Dissipation

Ingredients:

Binary Brackets (Poisson and Dissipative) + Generators

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

If $((\cdot, \cdot))$ Leibniz & bilinear

$$\dot{z}^i = J^{ij} \frac{\partial H}{\partial z^j} + G^{ij} \frac{\partial \mathcal{F}}{\partial z_j}$$

where

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

What is \mathcal{F} and what are the algebraic properties of $((\cdot, \cdot))$?

Metriplectic 2-Bracket

(pjm 1984,1984,1986)

- (f, g) symmetric, bilinear, appropriately degenerate
- Casimirs of noncanonical PB $\{, \}$ are 'candidate' entropies. Election of particular $S \in \{\text{Casimirs}\} \Rightarrow$ thermodynamic equilibrium (relaxed) state.

- Generator: $\mathcal{F} = H + S \quad \leftarrow$ "Free Energy"

- 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 $(H, f) = 0 \forall f \in C^\infty(\mathcal{Z})$.

- 2nd Law: entropy production

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

Lyapunov relaxation to the equilibrium state. Dynamics solves the equilibrium variational principle: $\delta\mathcal{F} = \delta(H + S) = 0$.

Metriplectic 4-Bracket Reduction to 2-Bracket

Symmetric 2-bracket:

$$(f, g)_H = (f, H; g, H) = (g, f)_H$$

Dissipative dynamics:

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

Energy conservation:

$$(g, H)_H = (H, g)_H = 0 \quad \forall g.$$

Entropy dynamics:

$$\dot{S} = (S, S)_H = (S, H; S, H) \geq 0$$

Metriplectic 4-brackets \rightarrow metriplectic 2-brackets of 1984, 1986!

Metriplectic 4-Bracket: Encompassing Definition of Dissipation

- Lots of geometry on Poisson manifolds with metric or connection. Emerges naturally.
- If Riemannian, entropy production rate is positive contravariant sectional curvature. For $\sigma, \eta \in \Lambda^1(\mathcal{Z})$, entropy production by

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

where the second equality follows if $\sigma = dS$ and $\eta = dH$.

Binary Brackets for Dissipation circa 1980 →

- Symmetric Bilinear Brackets (pjm 1980 → ..., IFS report 1983, published 1984 reduced MHD)
- Antisymmetric Bracket (possibly degenerate) (Kaufman and pjw 1982)
- Metriplectic Dynamics (pjm 1984, 1984, 1986, ... Kaufman 1984 had no degeneracy)
- Double Brackets (Vallis, Carnevale, Young, Shepherd; Brockett, Bloch ... 1989)
- GENERIC (Grmela 1984, with Oettinger 1997, ...) Binary but **not** Symmetric and **not** Bilinear \Leftrightarrow Metriplectic Dynamics!

4-Bracket Reduction to K-M Brackets

(Kaufman and Morrison 1982)

K-M done for plasma quasilinear theory.

Dynamics:

$$\dot{z} = [z, H]_S = (z, H; S, H)$$

Bracket Properties:

$$[f, g]_S = (f, g; S, H)$$

- bilinear
- antisymmetric, possibly degenerate
- energy conservation and entropy production

$$\dot{H} = [H, H]_S = 0 \quad \text{and} \quad \dot{S} = [S, H]_S \geq 0 \quad \Rightarrow \quad z \mapsto z_{eq}$$

4-Bracket Reduction to Double Brackets

(Vallis, Carnevale; Brockett, Bloch ... 1989)

Interchanging the role of H with a Casimir S :

$$(f, g)_S = (f, S; g, S)$$

Can show with assumptions

$$(C, g)_S = (C, S; g, S) = 0$$

for any Casimir C . Therefore $\dot{C} = 0$.

Practical tool for equilibria computation → Beautiful geometry with Fernandes-Koszul connection!

4-Bracket Reduction to 2-Brackets \equiv GENERIC

(Grmela 1984, with Öttinger 1997)

- Grmela 1984 bracket for Boltzmann not bilinear and not symmetric, unlike metriplectic 2-bracket.

GENERIC Vector Field in terms of dissipation function $\Xi(z, z_*)$:

$$\dot{z}^i = Y_S^i = \left. \frac{\partial \Xi(z, z_*)}{\partial z_{*i}} \right|_{z_* = \partial S / \partial z} .$$

Special Case:

$$\Xi(z, z_*) = \frac{1}{2} \frac{\partial S}{\partial z^i} G^{ij}(z) \frac{\partial S}{\partial z^j} \quad \Rightarrow \quad \dot{z}^i = Y_S^i = G^{ij}(z) \frac{\partial S}{\partial z^j} ,$$

- General Case: there exists a bracket and procedure (pjm & Updike) for linearizing and symmetrizing \Rightarrow

GENERIC (1997) \equiv Metriplectic (1984,1986)!

Existence – General Constructions

- For any Riemannian manifold \exists 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.
- Methods of construction? We describe two: Kulkarni-Nomizu and Lie algebra based. Goal is to develop intuition like building Lagrangians.

Construction via Kulkarni-Nomizu Product

Given σ and μ , two symmetric rank-2 tensor fields operating on 1-forms (assumed exact) df, dk and dg, dn , the K-N product is

$$\begin{aligned}\sigma \otimes \mu (df, dk, dg, dn) &= \sigma(df, dg) \mu(dk, dn) \\ &- \sigma(df, dn) \mu(dk, dg) \\ &+ \mu(df, dg) \sigma(dk, dn) \\ &- \mu(df, dn) \sigma(dk, dg).\end{aligned}$$

Metriplectic 4-bracket:

$$(f, k; g, n) = \sigma \otimes \mu (df, dk, dg, dn).$$

In coordinates:

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

Lie Algebras and Lie-Poisson Brackets

Lie Algebras: Denoted \mathfrak{g} , is a vector space (over \mathbb{R}, \mathbb{C} , for us \mathbb{R}) with binary, bilinear product $[\cdot, \cdot]: \mathfrak{g} \times \mathfrak{g} \rightarrow \mathfrak{g}$. In basis $\{e_i\}$, $[e_i, e_j] = c_{ij}^k e_k$. Structure constants c_{ij}^k . For example $\mathfrak{so}(3)$, which has $A \times (B \times C) + B \times (C \times A) + C \times (A \times B) \equiv 0$.

Lie-Poisson Brackets: special noncanonical Poisson brackets associated with any Lie algebra, \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

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

Pairing $\langle \cdot, \cdot \rangle: \mathfrak{g}^* \times \mathfrak{g} \rightarrow \mathbb{R}$, z^i coordinates for \mathfrak{g}^* , and c_{ij}^k structure constants of \mathfrak{g} . Note

$$J^{ij} = c_{ij}^k z_k.$$

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.

- Covariant connection $\nabla: \mathfrak{X} \times \mathfrak{X} \rightarrow \mathfrak{X}$. A contravariant connection $D: \Lambda^1(\mathcal{Z}) \times \Lambda^1(\mathcal{Z}) \rightarrow \Lambda^1(\mathcal{Z})$ satisfying 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 $\alpha, \beta, \gamma \in \Lambda^1(\mathcal{Z})$, $f \in \Lambda^0(\mathcal{Z})$. Add a metric, build 4-bracket like curvature from connection.

Examples

- finite-dimensional
- $1+1$ fluid theory
- $3+1$ fluid theory
- kinetic theory

Free Rigid Body (pjm Physica D 1986)

Angular momenta (L^1, L^2, L^3) , Lie-Poisson bracket with Lie algebra $\mathfrak{so}(3)$, $c_k^{ij} = -\epsilon_{ijk}$.

Hamiltonian:

$$H = \frac{(L^1)^2}{2I_1} + \frac{(L^2)^2}{2I_2} + \frac{(L^3)^2}{2I_3}$$

principal moments of inertia, I_i Casimir

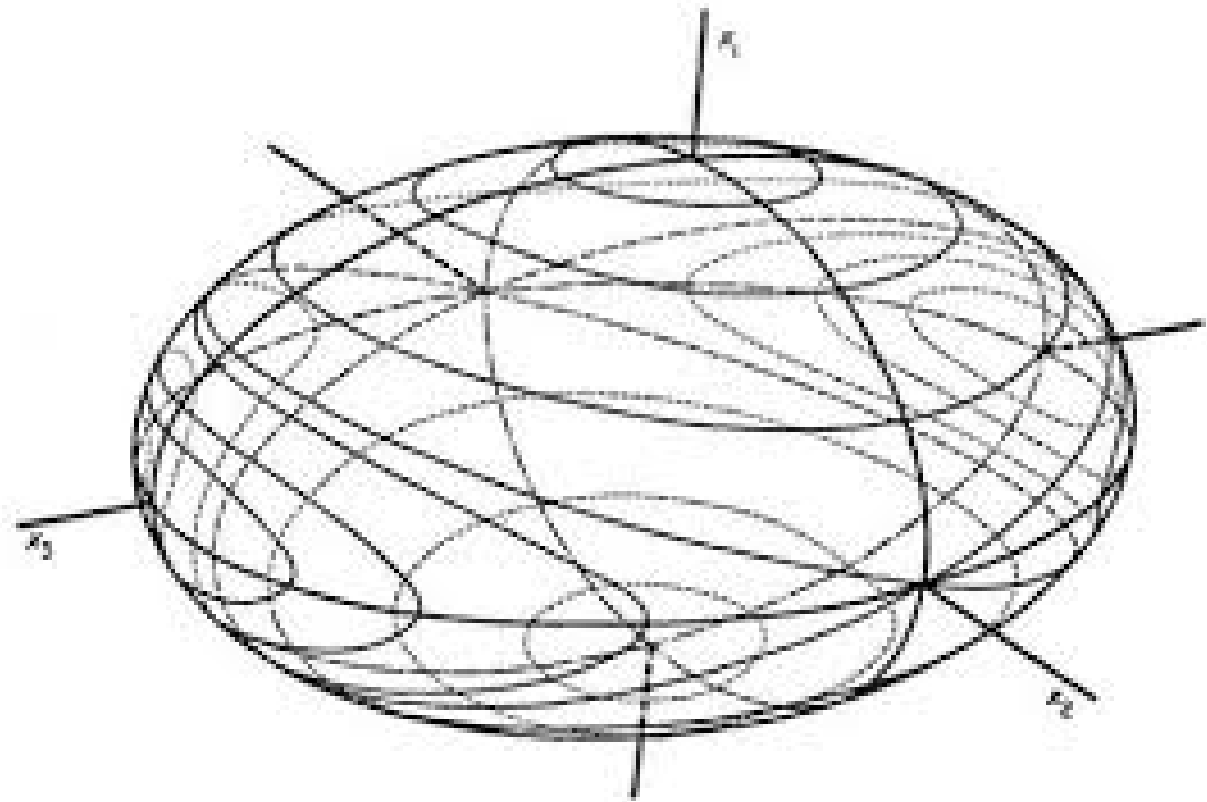
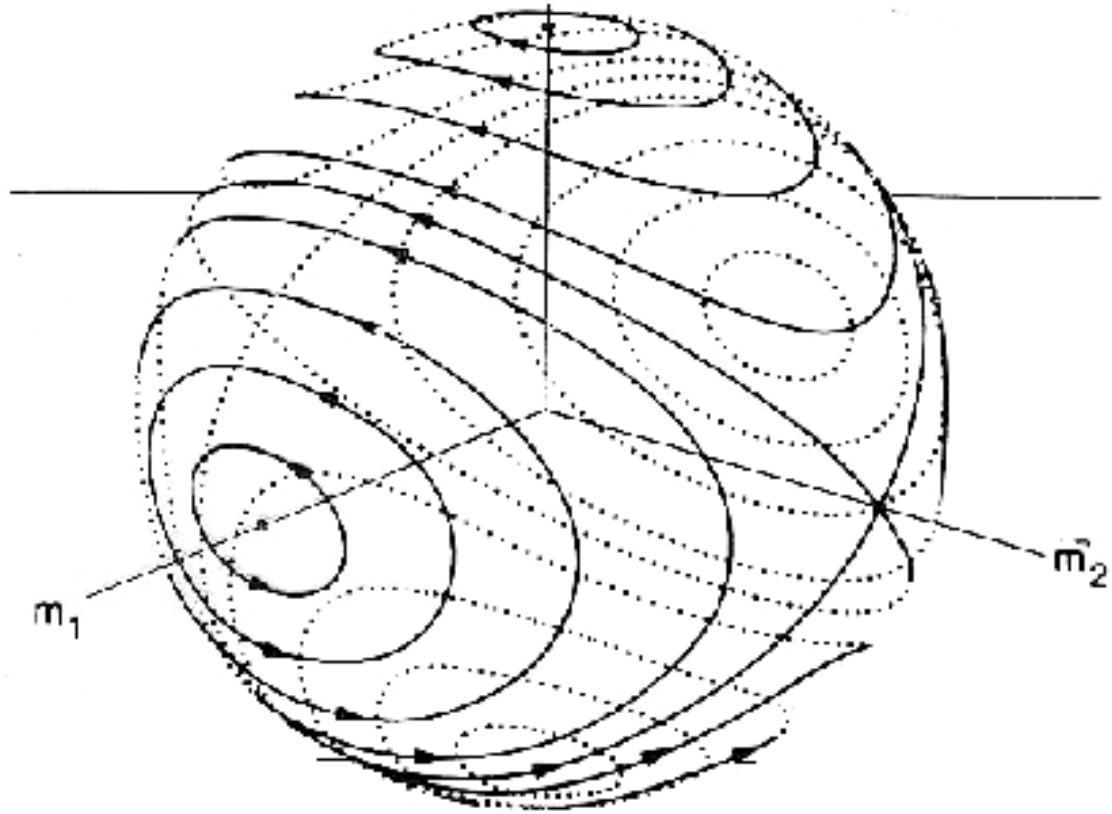
$$C = \|L\|^2 = (L^1)^2 + (L^2)^2 + (L^3)^2 = S,$$

Euler's equations:

$$\dot{L}^i = \{L^i, H\}$$

“Thermodynamics” \rightarrow design a system s.t. $\dot{H} = 0$ and $\dot{S} \geq 0$ (or $\dot{S} \leq 0$).

“Thermodynamical” Free Rigid Body (cont)



Growing entropy sphere $\dot{S} \geq 0$ at fixed energy ellipsoid $\dot{H} = 0$

“Thermodynamical” Free Rigid Body (cont)²

Use K-N product. Choose $\sigma^{ij} = \mu^{ij} = g^{ij} \Rightarrow$

$$R^{ijkl} = K (g^{ik} g^{jl} - g^{il} g^{jk}) ,$$

Riemannian *space form* with constant sectional curvature K .

Assume Euclidean gives metriplectic 4-bracket:

$$(f, k; g, n) = K (\delta^{ik} \delta^{jl} - \delta^{il} \delta^{jk}) \frac{\partial f}{\partial z^i} \frac{\partial k}{\partial z^j} \frac{\partial g}{\partial z^k} \frac{\partial n}{\partial z^l} ,$$

Metriplectic 2-bracket:

$$(f, g)_H = (f, H; g, H)$$

Precisely bracket and dynamics of pjm 1986!

$$\dot{L}^i = \{L^i, H\} + (L^i, S)_H = \{L^i, H\} + (L^i, H; S, H)$$

Infinite Dimensions – Field Theories $\partial f/\partial z \rightarrow \delta F/\delta\chi$

Multi-component fields:

$$\chi(z, t) = (\chi^1(z, t), \chi^2(z, t), \dots, \chi^M(z, t)), \quad z \in \mathcal{D}$$

Metriplectic 4-bracket:

$$(F, G; K, N) = \int d^N z \int d^N z' \int d^N z'' \int d^N z''' \hat{R}^{ijkl}(z, z', z'', z''') \\ \times \frac{\delta F}{\delta \chi^i(z)} \frac{\delta G}{\delta \chi^j(z')} \frac{\delta K}{\delta \chi^k(z'')} \frac{\delta N}{\delta \chi^l(z'''')}$$

Fréchet derivative:

$$\delta F[\chi; \eta] = \left. \frac{d}{d\epsilon} F[\chi + \epsilon\eta] \right|_{\epsilon=0} = \int_{\mathcal{D}} d^N z \frac{\delta F[\chi]}{\delta \chi^i} \eta^i$$

$\delta F/\delta\chi$ the functional (variational) derivative (a gradient)

$\hat{R}^{ijkl}(z, z', z'', z''')$ defined as distribution, an operator (e.g. a pseudo-differential ...) acting on the functional derivatives.

1D fluid $u(x, t)$: 1 + 1 + (1) Field Theory

Again use K-N product with operators Σ and M

$$(F, K; G, N) = \int_{\mathbb{R}} dx W \left(\Sigma(F_u, G_u) M(K_u, N_u) - \Sigma(F_u, N_u) M(K_u, G_u) + M(F_u, G_u) \Sigma(K_u, N_u) - M(F_u, N_u) \Sigma(K_u, G_u) \right),$$

W a constant and $F_u = \delta F / \delta u$, etc.

Choose

$$M(F_u, G_u) = F_u G_u$$

$$\Sigma(F_u, G_u)(x) = \partial F_u(x) \mathcal{H}[G_u](x) + \partial G_u(x) \mathcal{H}[F_u](x),$$

$\partial = \partial / \partial x$ and \mathcal{H} the Hilbert transform \Rightarrow

$$(F, G)_H = (F, H; G, H) = \int_{\mathbb{R}} dx W \left(\partial F_u \mathcal{H}[G_u] + \partial G_u \mathcal{H}[F_u] \right).$$

$$u_t = \dots (u, S)_H = -2W \mathcal{H}[\partial u].$$

Ott & Sudan 1969 fluid model of electron Landau damping (Hammett-Perkins 1990). $\mathcal{H} \rightarrow \partial \Rightarrow$ viscous dissipation

Thermodynamic Navier-Stokes (Eckart, 1940) $\chi = \{\rho, \sigma = \rho s, M = \rho v\}$

K-N again:

$$M(F_\chi, G_\chi) = F_\sigma G_\sigma$$

$$\Sigma(F_\chi, G_\chi) = \hat{\Lambda}_{ijkl} \partial_j F_{M_i} \partial_k G_{M_l} + a \nabla F_\sigma \cdot \nabla G_\sigma$$

$\partial_i := \partial/\partial x^i$ with general isotropic Cartesian tensor of order 4

$$\hat{\Lambda}_{ikst} = \alpha \delta_{ik} \delta_{st} + \beta (\delta_{is} \delta_{kt} + \delta_{it} \delta_{ks}) + \gamma (\delta_{is} \delta_{kt} - \delta_{it} \delta_{ks})$$

Construct

$$(F, G)_H = (F, H; G, H) \rightarrow \chi_t = \{\chi, H\} + (\chi, S)_H \Rightarrow$$

using $S = \int d^3x \rho s$ and $H = \int d^3x (\rho |v|^2/2 + \rho U(\rho, s))$

$$\partial_t v = -v \cdot \nabla v - \frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot \mathcal{T} \quad \leftarrow \mathcal{T} \text{ viscous stress}$$

$$\partial_t \rho = -\nabla \cdot (\rho v)$$

$$\partial_t s = -v \cdot \nabla s - \frac{1}{\rho T} \nabla \cdot \mathbf{q} + \frac{1}{\rho T} \mathcal{T} : \nabla v, \quad \mathbf{q} = -\kappa \nabla T$$

Reproduces pjm 1984!

Kinetic Theory Collision Operator

Phase space $z = (\mathbf{x}, \mathbf{v})$, density $f(z, t)$

Define operator on $w: \mathbb{R}^6 \rightarrow \mathbb{R}$ (at fixed time)

$$P[w]_i = \frac{\partial w(z)}{\partial v_i} - \frac{\partial w(z')}{\partial v'_i}$$

$$(F, K; G, N) = \int d^6 z \int d^6 z' \mathcal{G}(z, z') \\ \times (\delta \otimes \delta)_{ijkl} P[F_f]_i P[K_f]_j P[G_f]_k P[N_f]_l,$$

where simplest K-N

$$(\delta \otimes \delta)_{ijkl} = 2(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}).$$

with $S = - \int d^z f \ln f$

$$(f, H; SH) = ??$$

Landau-Lenard-Balescu collision operator!

Metriplectic 2-bracket $(f, g)_H$ in pjm 1984 again!

Final Comments

- See PJM & M. Updike, arXiv:2306.06787v2 [math-ph] for many more examples, finite and infinite.
- Useful for thermodynamically consistent model building, e.g., multiphase flow (Navier-Stokes-Cahn-Hilliard) with many constitutive relation effects (with A. Zaidni) and inhomogeneous collision operators for plasma (with N. Sato).
- Given that double brackets and metriplectic brackets have been used for computation of equilibria, metriplectic 4-bracket can be a new tool for equilibria. ← Easy to maintain R^{ijkl} symmetries in semi-discrete projection.
- New kind of structure to preserve: Symplectic, Poisson, FEEC, metriplectic 2-bracket, metriplectic 4-bracket?

Existing Computational Uses

- Poisson Integrators: symplectic on leaf and exact leaf preservation; GEMPIC, Kraus et al. for Vlasov-Maxwell system. B. Jayawardana, P. J. Morrison, and T. Ohsawa, Clebsch Canonization of Lie–Poisson Systems, J. Geometric Mechanics 14, 635 (2022).

Dynamical extremization with constraints:

- Simulated Annealing: Double brackets for equilibria
- Metriplectic relaxation

Double Bracket for Vortex States 1989

Good Idea:

Vallis, Carnevale, and Young, Shepherd (1989,1990)

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

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: Except only works sometimes, e.g., limited to circular vortex states

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.

Coordinates:

$$\dot{z}^i = ((z^i, H)) = J^{ik} g_{kl} J^{jl} \frac{\partial H}{\partial z^j}$$

symmetric, definite, and kernel of J .

$$\dot{C} = 0 \quad \text{with} \quad \dot{H} \leq 0$$

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 .

Our New Idea:

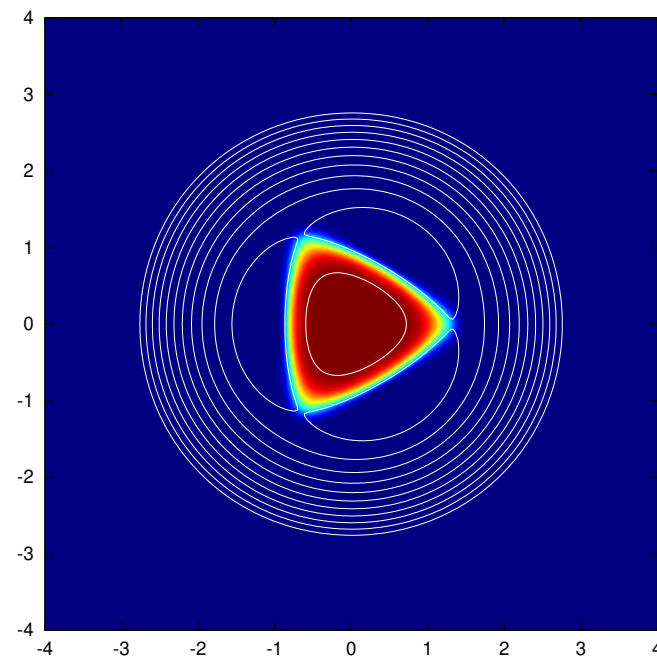
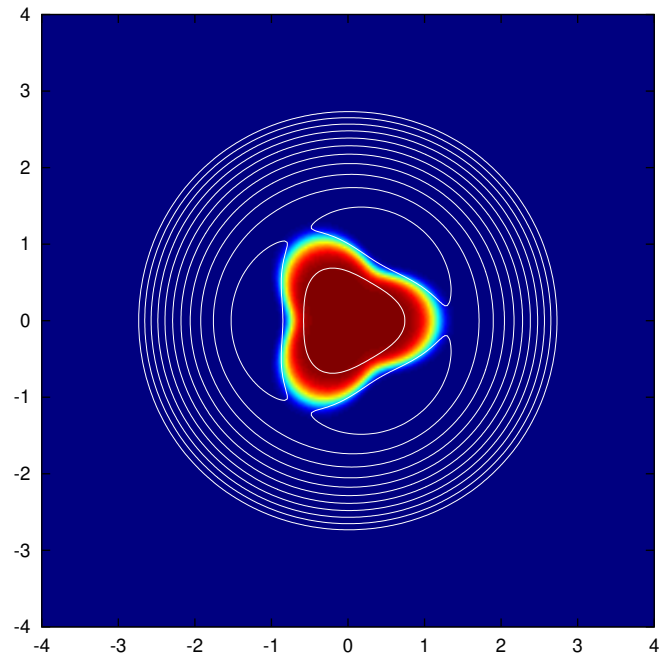
Do simulated Annealing with Generalized Dirac Bracket

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

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

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

2D Euler Vortex States (Flierl and pjm 2011)



Vorticity contours. The three-fold symmetric initial condition finds tri-polar state using Dirac bracket Simulated Annealing.

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

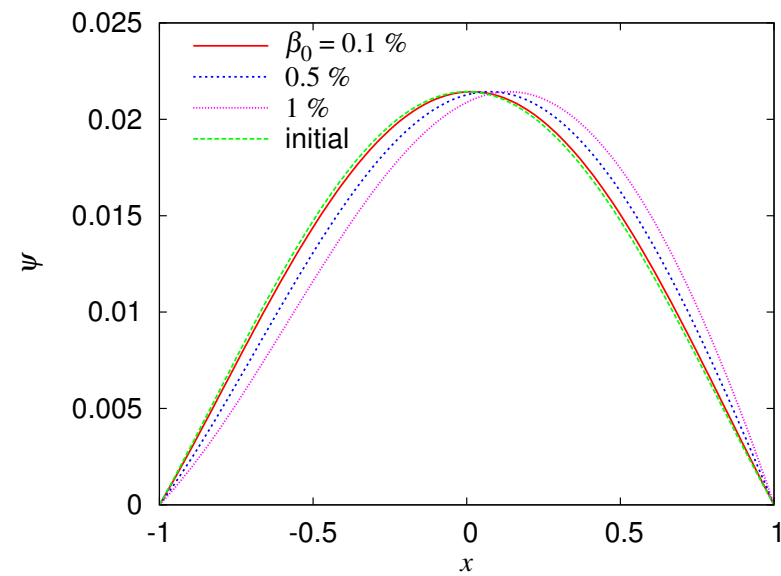
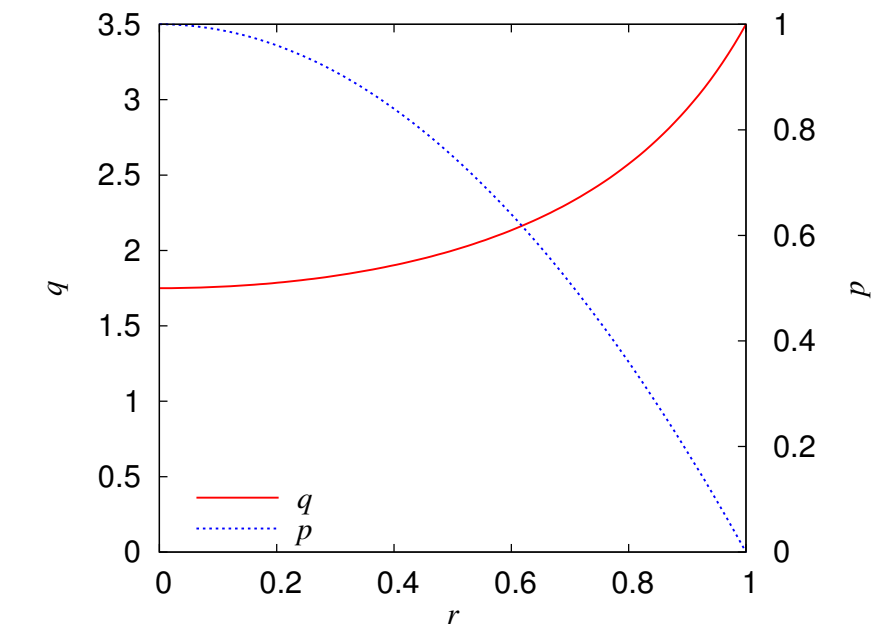
$$\begin{aligned}\frac{\partial U}{\partial t} &= [U, \varphi] + [\psi, J] - \epsilon \frac{\partial J}{\partial \zeta} + [P, h] \\ \frac{\partial \psi}{\partial t} &= [\psi, \varphi] - \epsilon \frac{\partial \varphi}{\partial \zeta} \\ \frac{\partial P}{\partial t} &= [P, \varphi]\end{aligned}$$

Extremization

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

C s Casimirs and P s dynamical invariants.

Sample Double Bracket SA equilibria



Nested Tori are level sets of ψ ; q gives pitch of helical 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 it is an energy extremum and must be stable

Sample Double Bracket SA unstable equilibria

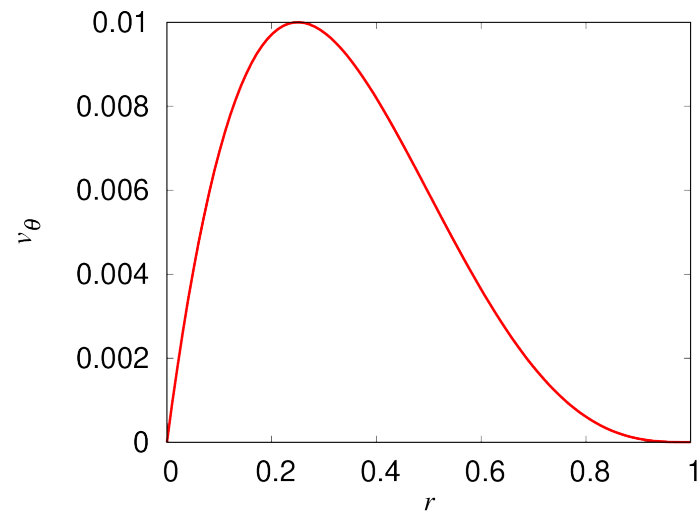
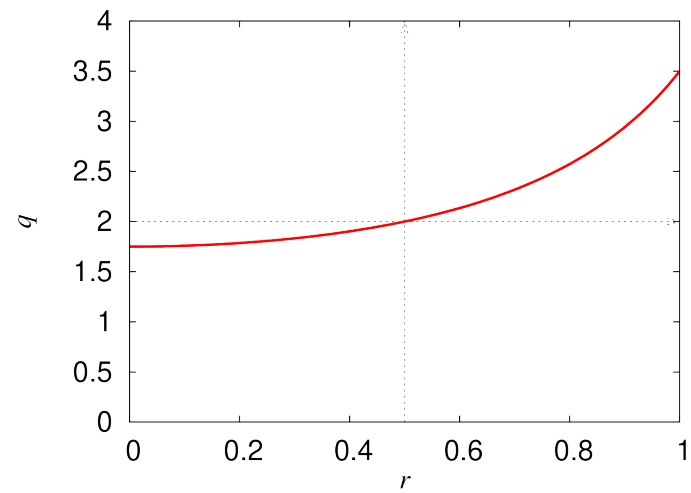
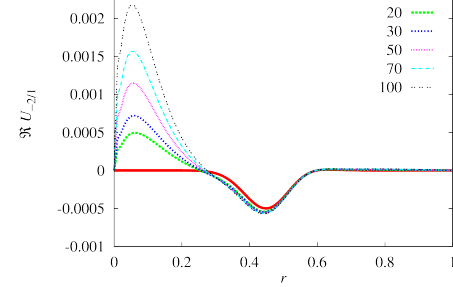
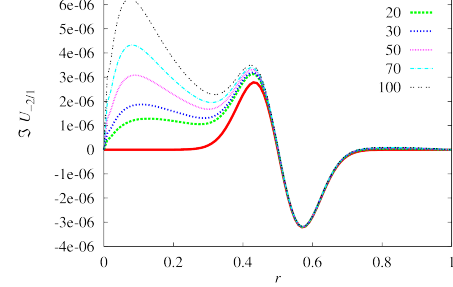


FIG. 12: Poloidal rotation velocity v_θ profile.

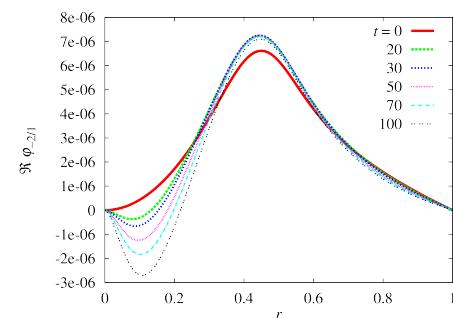




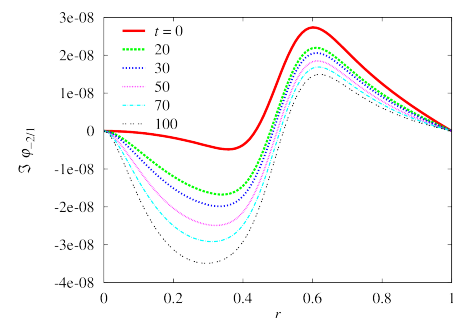
(a) Radial profile of $\Re U_{-2,1}$.



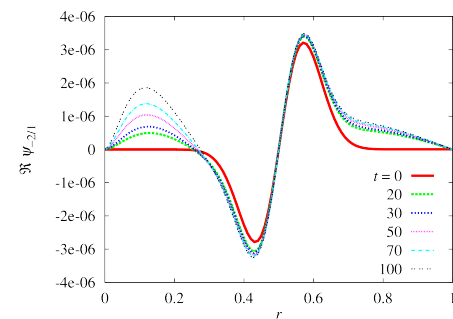
(b) Radial profile of $\Im U_{-2,1}$.



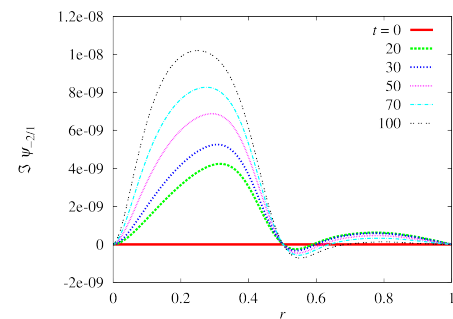
(c) Radial profile of $\Re \varphi_{-2,1}$.



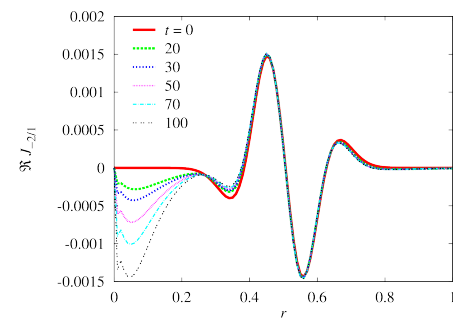
(d) Radial profile of $\Im \varphi_{-2,1}$.



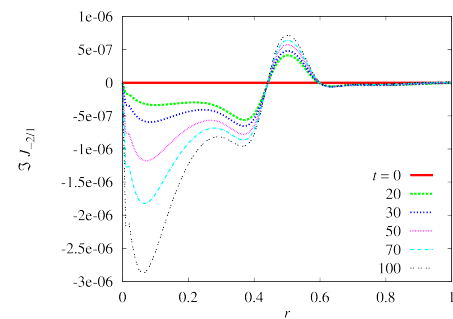
(e) Radial profile of $\Re \psi_{-2,1}$.



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



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



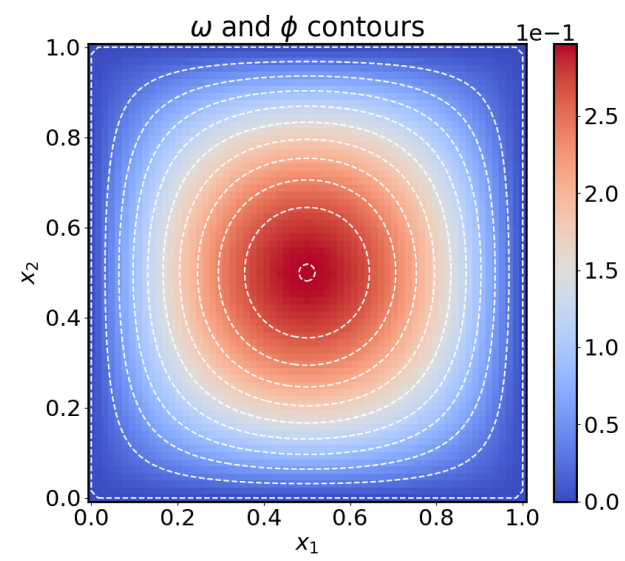
(h) Radial profile of $\Im J_{-2,1}$.

Metriplectic Simulated Annealing.

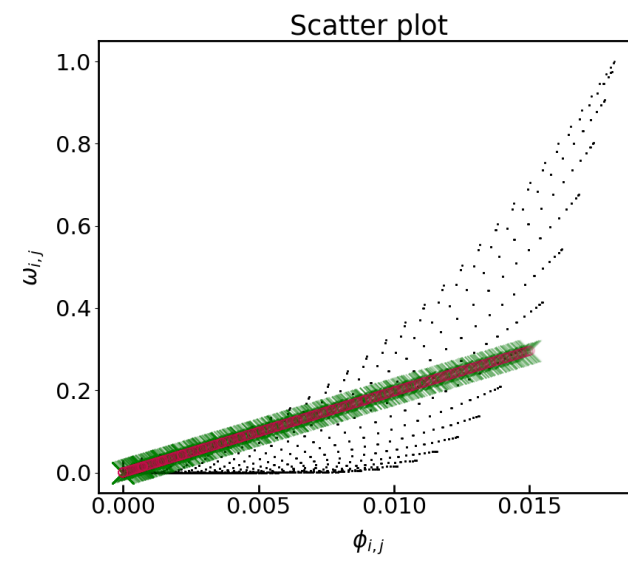
Camilla Bressen Ph.D.

TUM & Max Planck, Garching, Germany

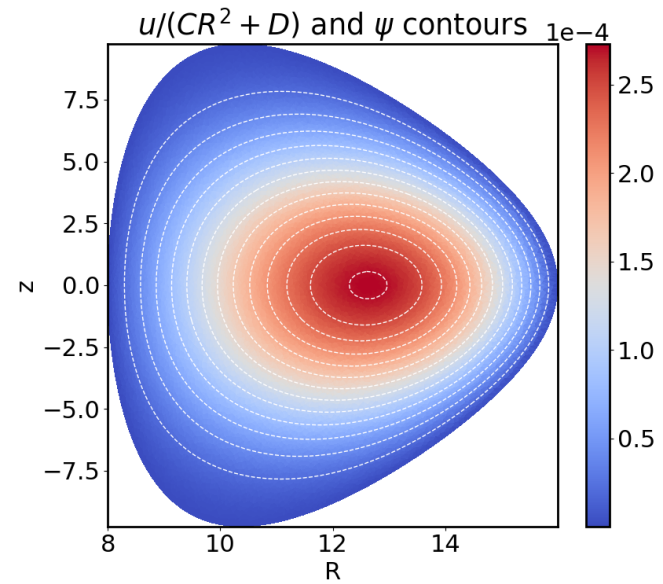
Vortex states and MHD equilibria



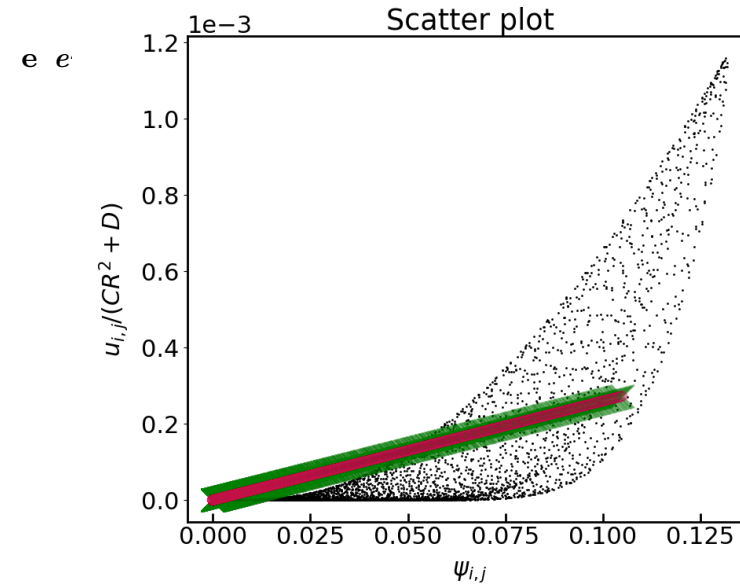
(a) Color plot.



(b) Scatter plot.



(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.

Computation Summary

- Poisson Integrators
- Dirac Double Bracket Simulated Annealing for Equilibria and Stability
- Metriplectic Simulated Annealing for Equilibria

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