Metriplectic 4-bracket dynamics: the natural way to build in thermodynamic consistency

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Geometry of metriplectic 4-brackets: with Michael Updike

pjm & M. Updike, arXiv:2306.06787v1 [math-ph] 11 Jun 2023.

→ **Theory of thermodynamically consistent theories!**

Theories & Models $\rightarrow$ Dynamics

Goal:
Predict the future or explain the past $\Rightarrow$

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

A dynamical system. 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:

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

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

General Dissipation:

$$V_D = ?\ldots \qquad \rightarrow \qquad V_D = G\,\frac{\partial F}{\partial z}$$

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*.

Cahn-Hilliard (1958): $\frac{\partial n}{\partial t} = \nabla^2 \frac{\delta \mathcal{F}}{\delta n} = \nabla^2 \left(n^3 - n - \nabla^2 n\right)$
Phase separation, nonlinear diffusive dissipation, binary fluid ..

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

Hamilton's Canonical Equations

Phase Space with Canonical Coordinates: (q, p)

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

Equations of Motion:

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

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

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

$J_c :=$ <u>Poisson tensor</u>, 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 $\longrightarrow$ $\{f, \{g, h\}\} + \{b, \{h, f\}\} + \{h, \{f, g\}\} = 0$

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

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

Sophus Lie: $detJ = 0 \Longrightarrow$ Canonical Coordinates plus Casimirs

(Lie's distinguished functions!)

Poisson Brackets – Flows on Poisson Manifolds

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

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

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 $\boldsymbol{d}$ exterior derivative.

$$\{f,g\} = J(\boldsymbol{d}f \wedge \boldsymbol{d}g) = \langle \boldsymbol{d}f, J\boldsymbol{d}g\rangle = J(\boldsymbol{d}f, \boldsymbol{d}g)\,.$$

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

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

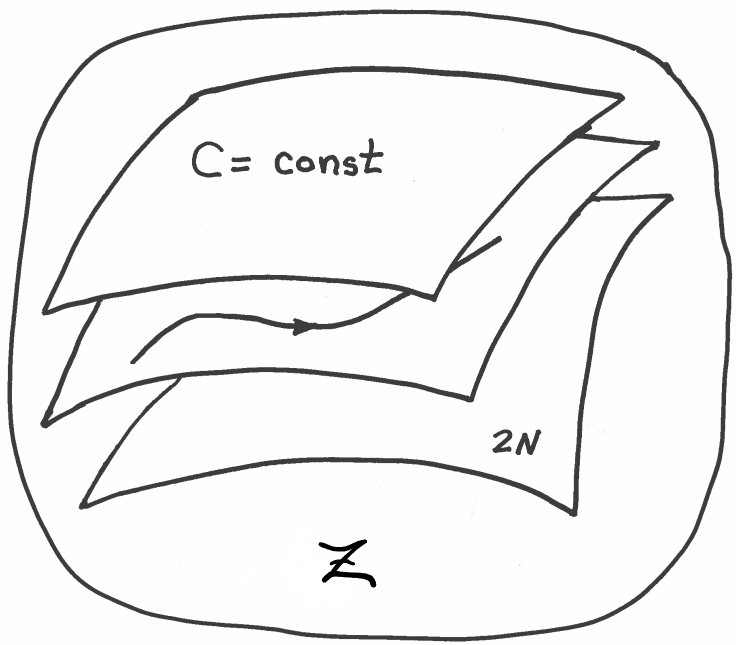
Because of degeneracy, $\exists$ functions C st $\{f, C\} = 0$ for all $f \in C^\infty(\mathcal{Z})$. Casimir invariants (Lie's distinguished functions!).

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:



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 <u>multilinear</u>.

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

$$(f, k; g, n) := R(\boldsymbol{d}f, \boldsymbol{d}k, \boldsymbol{d}g, \boldsymbol{d}n)\,,$$

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

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

• 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) linearity in all arguments, e.g,

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

(ii) algebraic identities/symmetries

$$\begin{aligned}
(f,k;g,n) &= -(k,f;g,n) \\
(f,k;g,n) &= -(f,k;n,g) \\
(f,k;g,n) &= (g,n;f,k) \\
(f,k;g,n) &+ (f,g;n,k) + (f,n;k,g) = 0 \qquad \leftarrow \text{not needed}
\end{aligned}$$

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

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

which is manifest when written 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.

Early 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

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

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

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: $\mathcal{F} = H + S \qquad \leftarrow$ "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:

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

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

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

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

Binary Brackets for Dissipation circa 1980 $\rightarrow$

- Symmetric Bilinear Brackets (pjm 1980 –. . . , IFS report 1983, published 1984 reduced MHD)

- Antisymmetric Bracket (possibly degenerate) (Kaufman and pjm 1982)

- Metriplectic Dynamics (pjm 1984, 1984, 1986, . . . Kaufman 1984 had no degeneracy)

- GENERIC (Grmela 1984, with Oettinger 1997, . . .) Binary but **not** Symmetric and **not** Bilinear $\Leftrightarrow$ Metriplectic Dynamics!

- Double Brackets (Vallis, Carnevale, Young, Shepherd; Brockett, Bloch ... 1989)

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 (Koszul construction)

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

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

Practical tool for equilibria computation $\rightarrow$ Beautiful geometry with Fernandes-Koszul connection!

4-Bracket Reduction to 2-Brackets ≡ 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:

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

• General Case: there exists a bracket and procedure (pjm & Updike) for linearizing and symmetrizing ⇒

$$\boxed{\text{GENERIC (1997)} \equiv \text{Metriplectic (1984,1986)!}}$$

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) $\boldsymbol{d}f, \boldsymbol{d}k$ 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:

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

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 $[\cdot,\cdot]\colon \mathfrak{g}\times\mathfrak{g} \to \mathfrak{g}$. 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 $\boldsymbol{A}\times(\boldsymbol{B}\times\boldsymbol{C}) + \boldsymbol{B}\times(\boldsymbol{C}\times\boldsymbol{A}) + \boldsymbol{C}\times(\boldsymbol{A}\times\boldsymbol{B}) \equiv 0$.

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

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

Pairing $<\ ,\ >\colon \mathfrak{g}^*\times\mathfrak{g} \to \mathbb{R}$, 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.

Examples

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

Free Rigid Body

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

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

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

Euler's equations:

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

"Thermodynamics" $\rightarrow$ design a system s.t. $\dot{H} = 0$ and $\dot{S} \leq 0$.

“Thermodynamical” Free Rigid Body

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

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

Riemannian *Space form* with constant sectional curvature K.

Assume Euclidean gives metriplectic 4-bracket:

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

Metriplectic 2-bracket:

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

Precisely bracket and dynamics of pjm 1986!

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

1D fluid $u(x,t)$

Again use K-N product with operators Σ and M

$$
\begin{aligned}
(F,K;G,N) \;=\; \int_{\mathbb{R}} dx\, W\Big(&\Sigma(F_u,G_u)M(K_u,N_u) \\
&-\Sigma(F_u,N_u)M(K_u,G_u)+M(F_u,G_u)\Sigma(K_u,N_u) \\
&-M(F_u,N_u)\Sigma(K_u,G_u)\Big)\,,
\end{aligned}
$$

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 $\Rightarrow$

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

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

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

Thermodynamic Navier-Stokes: $\chi = \{\rho, \sigma = \rho s, \boldsymbol{M} = \rho \boldsymbol{v}\}$

K-N again:

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

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

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

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

Construct

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

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

$$\partial_t \boldsymbol{v} = -\boldsymbol{v} \cdot \nabla \boldsymbol{v} - \frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla \cdot \mathcal{T}$$

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

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

Reproduces pjm 1984!

Collision Operator

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

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

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

$$\begin{aligned}(F,K;G,N) &= \int d^6z \int d^6z'\, \mathcal{G}(z,z') \\ &\quad \times\ (\delta \owedge \delta)_{ijkl}\, P\left[F_f\right]_i P\left[K_f\right]_j P\left[G_f\right]_k P\left[N_f\right]_l\,,\end{aligned}$$

where simplest K-N

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

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!

Theory Final Comments

• See PJM & M. Updike, arXiv:2306.06787v1 [math-ph] 11 Jun 2023 for many more examples, finite and infinite.

• Useful for thermodynamically consistent model building, e.g., multiphase flow (Navier-Stokes-Cahn-Hiliard) with many constitutive relation effects (with A. Zaidni) and inhomogeneous collision operator (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.

• 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

$\boxed{\text{Use various bracket dynamics to effect extremization.}}$

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.

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

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:

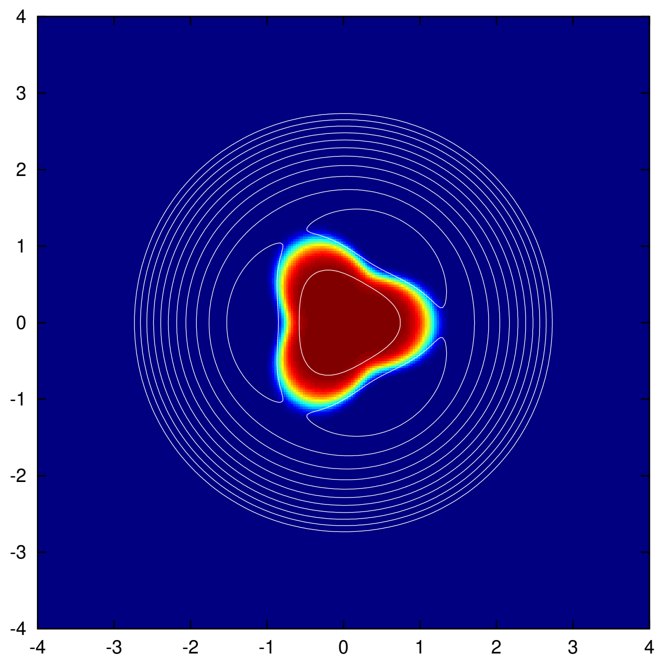
Do simulated Annealing with Generalized Dirac Bracket

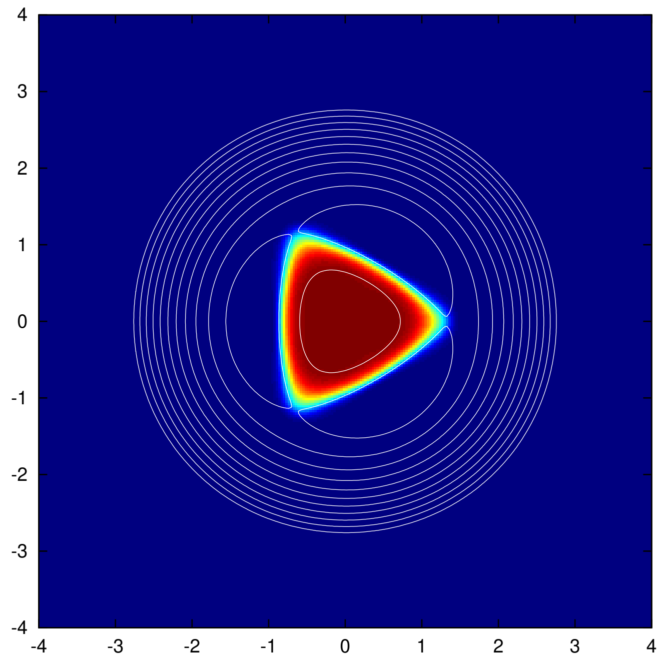
$$((F,G))_D = \int d\mathbf{x} d\mathbf{x}' \, \{F,\zeta(\mathbf{x})\}_D \; \mathcal{G}(\mathbf{x},\mathbf{x}') \; \{\zeta(\mathbf{x}'),G\}_D$$

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

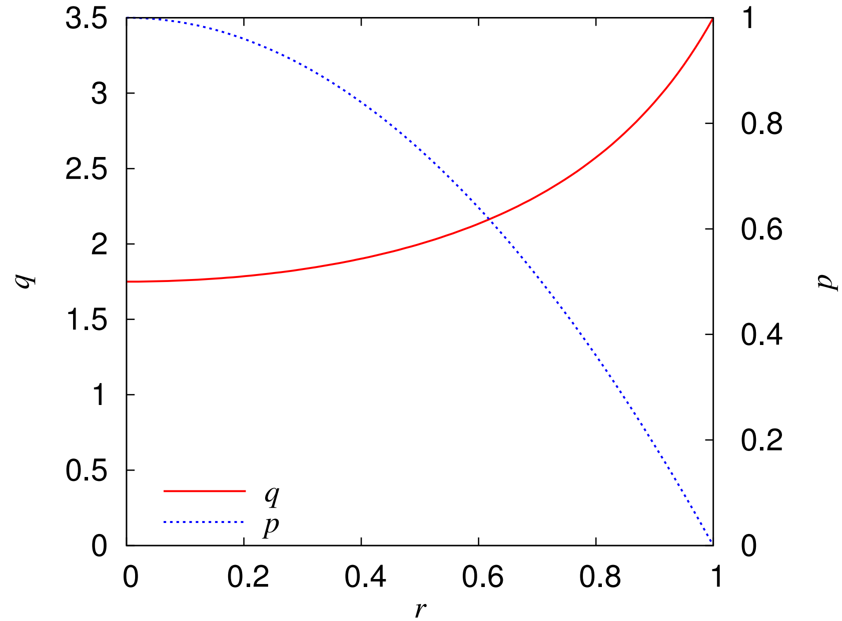
$$\begin{aligned}
\frac{\partial U}{\partial t} &= [U, \varphi] + [\psi, J] - \epsilon \frac{\partial J}{\partial \zeta} + [P, h] \\
\frac{\partial \psi}{\partial t} &= [\psi, \varphi] - \epsilon \frac{\partial \varphi}{\partial \zeta} \\
\frac{\partial P}{\partial t} &= [P, \varphi]
\end{aligned}$$

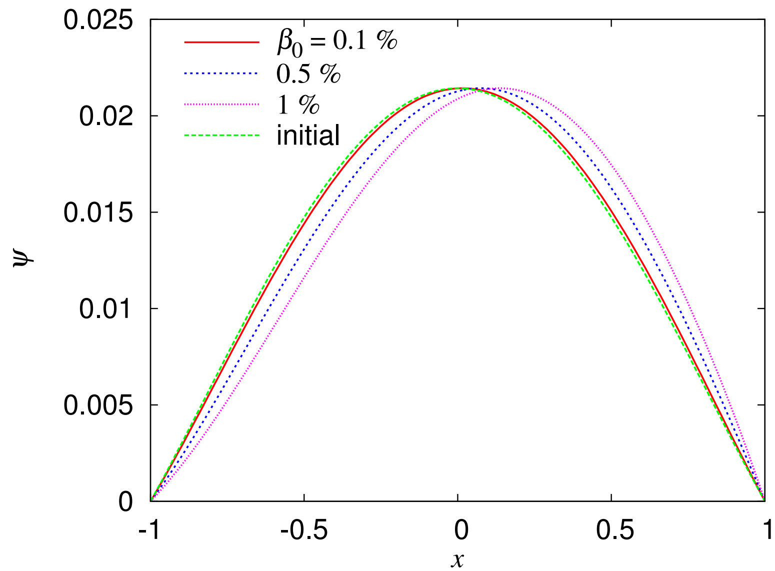
Extremization

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

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

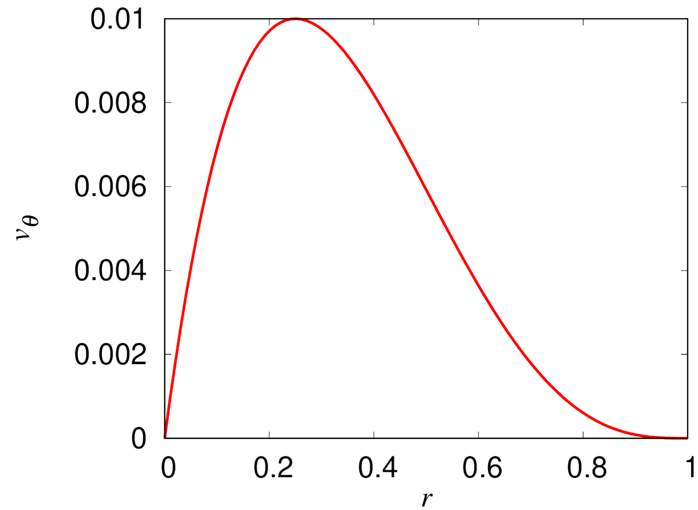
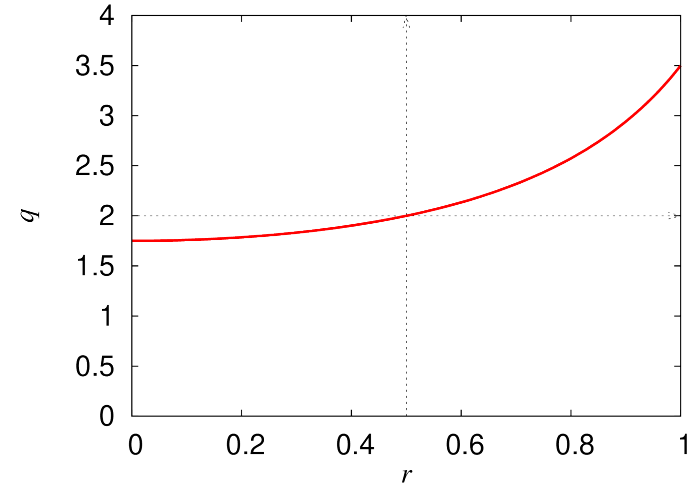
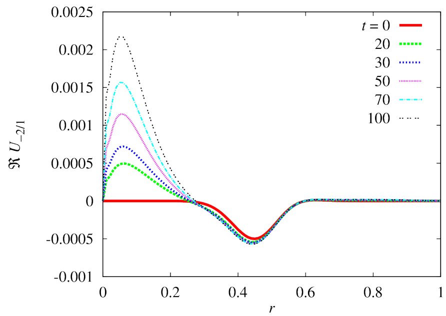
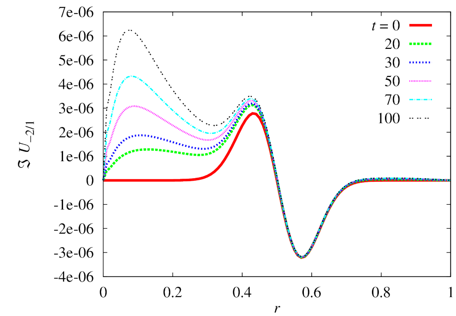


FIG. 12: Poloidal rotation velocity v_θ profile.

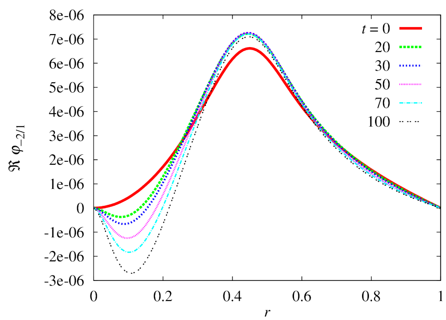




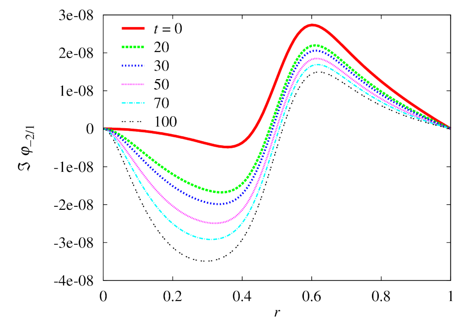
(a) Radial profile of $\Re U_{-2,1}$.



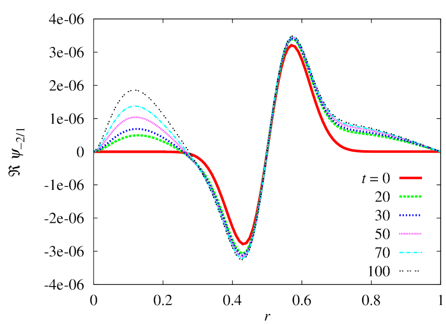
(b) Radial profile of $\Im U_{-2,1}$.



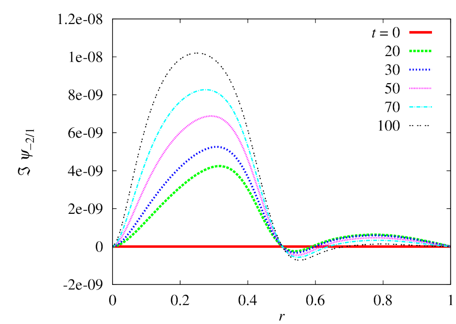
(c) Radial profile of $\Re \varphi_{-2,1}$.



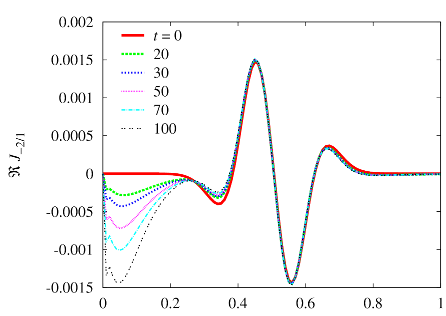
(d) Radial profile of $\Im \varphi_{-2,1}$.



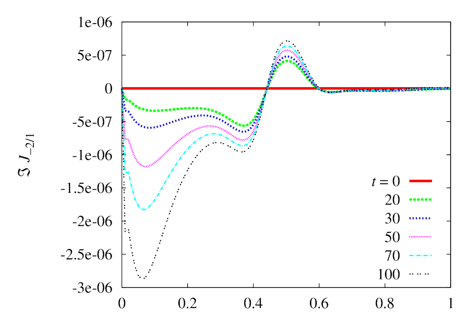
(e) Radial profile of $\Re \psi_{-2,1}$.



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



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

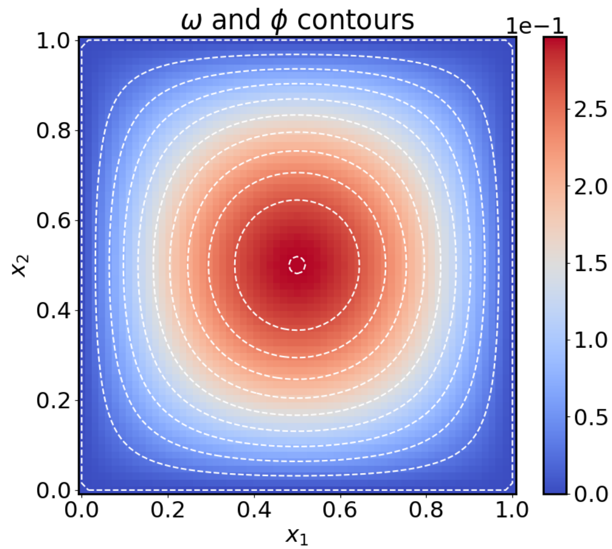


(h) Radial profile of $\Im J_{-2,1}$.

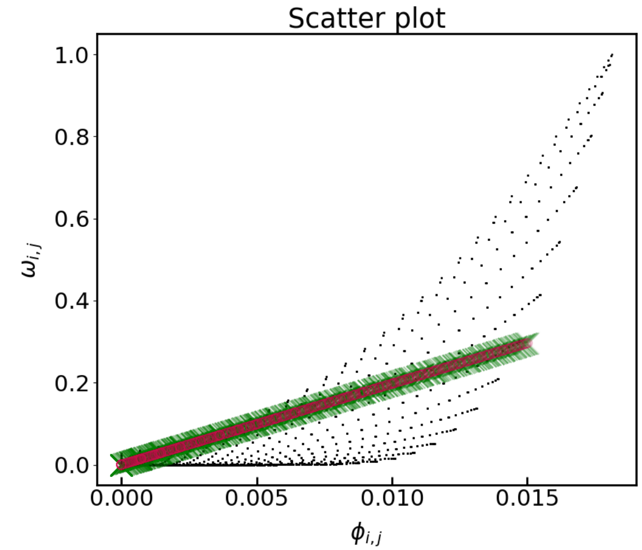
Metriplectic Simulated Annealing.

Camilla Bressen Ph.D.
TUM & Max Planck, Garching, Germany

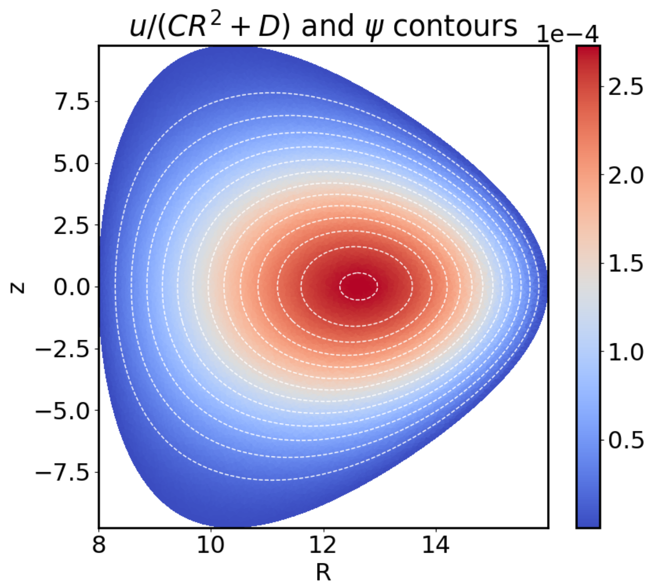
Vortex states and MHD equilibria



(a) Color plot.

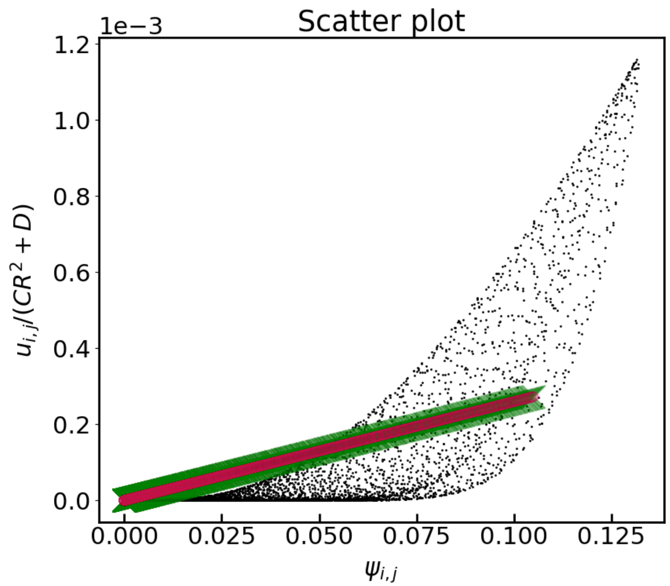


(b) Scatter plot.



e *e*

(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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