Unified Thermodynamic Algorithm (UTA) for constructing thermodynamically consistent systems via the metriplectic 4-bracket and its application.

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Overview:

- Metriplectic 4-bracket theory of thermodynamically consistent theories.
- UTA, an algorithm for constructing such theories.
- Use UTA to construct consistent Navier-Stokes-Fourier (a pedagogical example).
- Mention numerical implementation for Navier-Stokes-Fourier

Old and New Papers

Old:

- A. N. Kaufman and P. J. Morrison, "Algebraic Structure of the Plasma Quasilinear Equations," Physics Letters A 88, 405–406 (1982).
- P. J. Morrison, "Bracket Formulation for Irreversible Classical Fields," Physics Letters A **100**, 423–427 (1984).
- P. J. Morrison, "Some Observations Regarding Brackets and Dissipation," arXiv:2403.14698v1 [mathph] 15 Mar 2024 (1984 CPAM report).
- P. J. Morrison, "A Paradigm for Joined Hamiltonian and Dissipative Systems," Physica D **18**, 410–419 (1986).

New:

- A. Zaidni, P. J. Morrison, and R. Boukharfane, "Metriplectic 4-Bracket Algorithm for Constructing Thermodynamically Consistent Dynamical Systems," Draft (2024)
- W. Barham, P. J. Morrison, and A. Zaidni, "A Thermodynamically Consistent Discretization of 1D Thermal-Fluid Models Using their Metriplectic 4-Bracket Structure," arXiv:2410.11045v2 [physics.comp-ph] 19 Oct 2024
- A. Zaidni, P. J. Morrison, and S. Benjelloun, "Thermodynamically Consistent Cahn-Hilliard-Navier-Stokes Equations Using the Metriplectic Dynamics Formalism," Physica D **468**, 134303 (11pp) (2024).
- N. Sato and P. J. Morrison, "A Collision Operator for Describing Dissipation in Noncanonical Phase Space," Fundamental Plasma Physics **10**, 100054 (18pp) (2024).
- P. J. Morrison and M. Updike, "Inclusive Curvature-Like Framework for Describing Dissipation: Metriplectic 4-Bracket Dynamics," Physical Review E **109**, 045202 (22pp) (2024).
- B. Coquinot and P. J. Morrison, "A General Metriplectic Framework with Application to Dissipative Extended Magnetohydrodynamics," Journal of Plasma Physics **86**, 835860302 (32pp) (2020).

Other related work: G. Flierl; O. Maj, C. Bressan, M. Krause; M. Furukawa

Confession

- Similar to talk in June, 2024 at NMPP, Garching
- Similar to talk in July, 2024 Stellarator Theory, Greifswald
- This talk has lots of equations!

What's New Since Previous Talks?

- Direct procedure for constructing the metriplectic 4-bracket. Completion of the UTA.

$$\text{Flux} - \text{Affinity Relation:} \qquad \boldsymbol{J}^\alpha = L^{\alpha\beta} X_\beta \quad \rightarrow \quad \boldsymbol{J}^\alpha = -L^{\alpha\beta}\,\nabla(\delta H/\delta\xi^\beta)$$

- First numerical implementation via 4-bracket discretization for 1-D Navier-Stokes-Fourier. Finite element projection of PDE to thermodynamically consistent finite-dimensional 4-bracket, i.e. ODEs. For example, for the density $\rho(x,t)$

$$\rho_h(x,t) = \sum_{i=1}^{N} \rho_i(t)\phi_i(x) \quad \rightarrow \quad \dot{\rho}_i(t) = \{\rho_i, H\} + (\rho_i, H; S, H) \ldots$$

Results use Firedrake library, implicit midpoint, Irksome module ...

What is structure? Why care?

Old Structure:

B-lines as area preserving (symplectic) maps (1952), adiabatic invariants (1960s), breaking of invariant tori (1970s), Lie transforms (1975) noncanonical guiding center (1980), noncanonical MHD and Vlasov (1980), noncanonical drift and gyrokinetics (1985) ...

New Structure:

FEEC, cohomology and homology, Poisson integrators, the metriplectic 4-bracket, ...

Yesterday's exotic structure is today's common place!

Thermodynamic Consistency – Examples

Navier-Stokes (**inconsistent**):

$$\partial_t \boldsymbol{v} = -\boldsymbol{v}\cdot\nabla\boldsymbol{v} - \frac{1}{\rho}\nabla p + \frac{1}{\rho}\nabla\cdot\mathcal{T} \qquad \leftarrow \; \mathcal{T} \text{ viscous stress tensor} \sim \nabla v$$

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

$$H = \int_\Omega \rho\,|\boldsymbol{v}|^2/2 + \rho u(\rho) \quad \text{and} \quad \dot{H} \neq 0$$

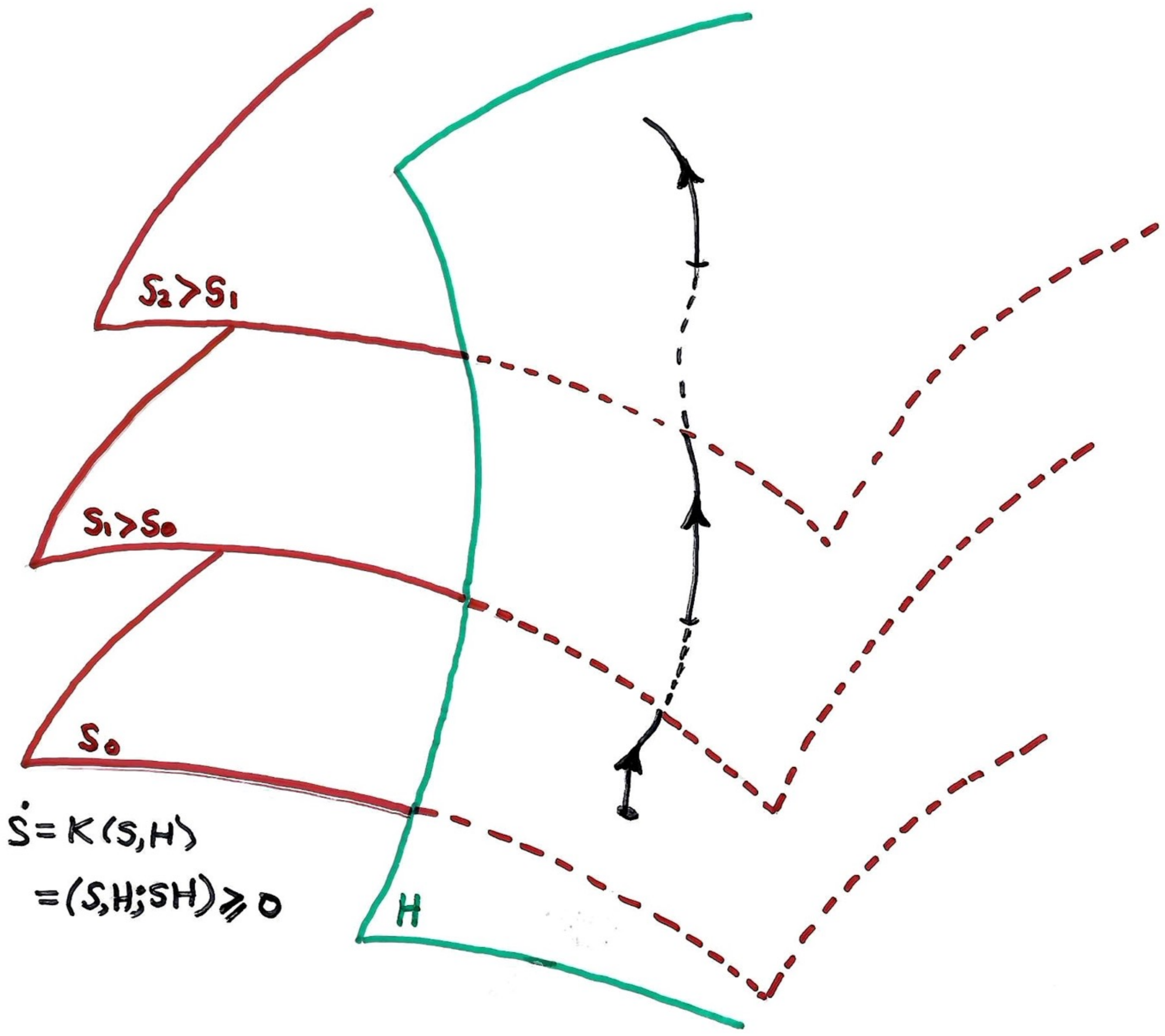
Navier-Stokes Fourier (**consistent**) (Eckart 1940):

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

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

$$\partial_t s = -\boldsymbol{v}\cdot\nabla s - \frac{1}{\rho T}\nabla\cdot\boldsymbol{q} + \frac{1}{\rho T}\mathcal{T} : \nabla\boldsymbol{v} \qquad \text{heat flux \& viscous heating}$$

$$H = \int_\Omega \rho\,|\boldsymbol{v}|^2/2 + \rho u(\rho, s)\,, \quad \dot{H} = 0 \quad \text{and} \quad S = \int_\Omega \rho s \;\rightarrow\; \dot{S} \geq 0$$



S2>S1
S1>S0
S0
H
Ṡ = K(S,H)
=(S,H;SH) ≥ 0

All Dynamical Models Have Vector Fields, $V(z)$

Natural Split:

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

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

General Hamiltonian Form:

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

where $J(z)$ is Poisson tensor/operator, $\{f, g\}$ Poisson bracket, and H is the Hamiltonian.

General Dissipation:

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

Build in thermodynamic consistency: 1st law Hamiltonian $\dot{H} = 0$ and 2nd law entropy $\dot{S} \geq 0$.

Building Theories - Traditional Physics Approach

Identify configuration space:

- Coordinates $q \in \mathcal{Q}$.
- Identify kinetic and potential energies, T and V.
- Construct Lagrangian:

$$\mathcal{L} = T - V\,.$$

- Obtain Lagrange's equations of motion:

$$\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} = 0\,.$$

For both finite systems and field theories consider symmetries, etc.

Unified Thermodynamic Algorithm - 4 Steps

1. Identify dynamical variables defined on $\Omega \subset \mathbb{R}^3$; e.g. for FNS

$$\Psi = (\boldsymbol{v}, \rho, s) \qquad \text{or} \qquad \boldsymbol{\xi} = (\boldsymbol{m} = \rho \boldsymbol{v}, \rho, \sigma = \rho s)$$

2. Propose energy and entropy functionals, $H[\Psi]$ and $S[\Psi]$; for FNS

$$H = \int_\Omega \frac{\rho}{2} |\mathbf{v}|^2 + \rho u(\rho, s) \quad \text{and} \quad S = \int_\Omega \rho s = \int_\Omega \sigma$$

3. Find Poisson bracket $\{F, G\}$ for which entropy S is a Casimir invariant, $\{F, S\} = 0 \, \forall \, F$

4. Construct metriplectic 4-bracket $(F, K; G, N)$ via Kulkarni-Nomizu product by a **new method that separates local thermodynamics from phenomenological quantities**, giving the EoMs as Poisson bracket + 4-bracket:

$$\partial_t \boldsymbol{\xi} = \{\boldsymbol{\xi}, H\} + (\boldsymbol{\xi}, H; S, H)$$

Result automatically Thermodynamically consistent!

Success of UTA

So far the method corrects or extends every case considered!

- Cahn-Hilliard-Navier-Stokes: agrees with Anderson et al.; corrects Guo and Lin

- Brenner-Navier-Stokes: UTA produces Brenner and Öttinger as special cases. Corrects their statements that their results are most general.

- Collisions on noncanonical phase space: Generalization of Landau for drift kinetic, ...

Hamiltonian Review

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

Hamilton's Canonical Equations

Phase Space with Canonical Coordinates: (q,p)

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

Equations of Motion:

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

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

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

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

Noncanonical Hamiltonian Structure

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

Noncanonical Coordinates:

$$\dot{z}^a = \{z^a, H\} = J^{ab}(z)\frac{\partial H}{\partial z^b}\,, \qquad a, b = 1, 2, \ldots M$$

Noncanonical Poisson Bracket:

$$\{f, g\} = \frac{\partial f}{\partial z^a} J^{ab}(z) \frac{\partial g}{\partial z^b}\,, \qquad J(z) \neq J_c$$

Poisson Bracket Properties:

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

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

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

Jean Gaston 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!)

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.

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

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

$$\dot{z}^a = J^{ab}(z)\frac{\partial H(z)}{\partial z^b}\,, \qquad \mathcal{Z}'s \text{ coordinate patch } z = (z^1, \dots, z^M)$$

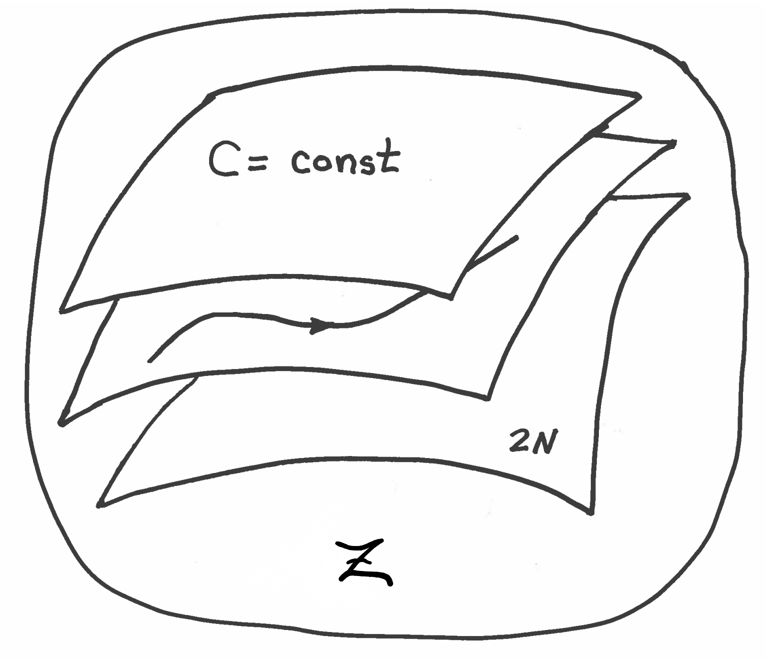
Because of degeneracy, $\exists$ functions C st $\{f, C\} = 0$ for all $f \in C^\infty(\mathcal{Z})$. Casimir invariants.

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:



3. Ideal Fluid Poisson Bracket Dynamics

Hamiltonian:

$$H = \int_\Omega \frac{\rho|\mathbf{v}|^2}{2} + \rho u\,(\rho, s)\;, \qquad T = \frac{\partial u}{\partial s}\,, \qquad p = \rho^2 \frac{\partial u}{\partial \rho}\,.$$

M-G Poisson Bracket:

$$\{F, G\} = -\int_\Omega \mathbf{m} \cdot [F_{\boldsymbol{m}} \cdot \nabla G_{\boldsymbol{m}} - G_{\boldsymbol{m}} \cdot \nabla F_{\boldsymbol{m}}] + \rho\,[F_{\boldsymbol{m}} \cdot \nabla G_\rho - G_{\boldsymbol{m}} \cdot \nabla F_\rho]$$
$$+ \sigma\,[F_{\boldsymbol{m}} \cdot \nabla G_\sigma - G_{\boldsymbol{m}} \cdot \nabla F_\sigma]\,.$$

Equations of Motion:

$$\partial_t \mathbf{v} = \{\boldsymbol{v}, H\} = -\boldsymbol{v} \cdot \nabla \boldsymbol{v} - \nabla p/\rho\,, \quad \partial_t \rho = \{\rho, H\} = -\nabla \cdot (\rho\, \boldsymbol{v})\,, \quad \partial_t \sigma = \{\sigma, H\} = -\nabla \cdot (\sigma\, \boldsymbol{v})\,.$$

Casimir:

$$S = \int_\Omega \rho s = \int_\Omega \sigma\,.$$

Note: $F_{\boldsymbol{m}} = \delta F / \delta \boldsymbol{m}$, etc., functional derivatives.

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

Metriplectic Dynamics:

$$\dot{\boldsymbol{\xi}} = \{\boldsymbol{\xi}, H\} + (\boldsymbol{\xi}, H; S, H)$$

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, $\mathcal{F} = H - \mathcal{T}S$, s.t. $\dot{H} = 0$ and $\dot{S} \geq 0$. Various generators have been tried.

- Provides natural reductions to other bilinear & binary brackets. This theory includes all others, e.g. metriplectic 2-bracket of 1984: $(F, G)_H = (F, H; G, H)$. Before a guess, now an algorithm!

- 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):

$$(\,\cdot\,,\,\cdot\,;\,\cdot\,,\,\cdot\,)\colon \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \times \Lambda^0(\mathcal{Z}) \to \Lambda^0(\mathcal{Z})$$

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:

$$(f, k; g, n) = R^{abcd}(z)\frac{\partial f}{\partial z^a}\frac{\partial k}{\partial z^b}\frac{\partial g}{\partial z^c}\frac{\partial n}{\partial z^d}\,. \qquad \leftarrow \text{quadravector?}$$

• A blend of my previous ideas: Two important functions H and S, symmetries, curvature idea, multilinear brackets.

• Manifolds with both Poisson tensor, J^{ab}, and compatible quadravector R^{abcd}, 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

$$\begin{aligned}(f,k;g,n) &= -(k,f;g,n)\\ (f,k;g,n) &= -(f,k;n,g)\\ (f,k;g,n) &= (g,n;f,k)\end{aligned}$$

(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.**

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? Two important ones: Kulkarni-Nomizu and Lie algebra based. Goal is to develop intuition like building Lagrangians. Now a procedure.

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:

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

4. K-N Metriplectic 4-Brackets for FNS

Possible Fluxes:

$$\boldsymbol{J}_\rho = -H_\sigma \left[L^{\rho\rho}\nabla H_\rho + L^{\rho \boldsymbol{m}} \!:\! \nabla H_{\boldsymbol{m}} + L^{\rho\sigma}\nabla H_\sigma\right]$$
$$\bar{J}_{\mathbf{m}} = -H_\sigma \left[L^{\boldsymbol{m}\rho}\cdot\nabla H_\rho + L^{\boldsymbol{m}\boldsymbol{m}} \!:\! \nabla H_{\boldsymbol{m}} + L^{\boldsymbol{m}\sigma}\cdot\nabla H_\sigma\right]$$
$$\boldsymbol{J}_s = -H_\sigma \left[L^{\sigma\rho}\nabla H_\rho + L^{\sigma \boldsymbol{m}}\nabla H_{\boldsymbol{m}} + L^{\sigma\sigma}\nabla H_\sigma\right]$$

Desired Fluxes:

$$\boldsymbol{J}_\rho = 0\,, \quad \bar{J}_{\mathbf{m}} = -\bar{\bar{\Lambda}} : \nabla \mathbf{v}\,, \quad \boldsymbol{J}_s = -\frac{\bar{\kappa}}{T}\cdot\nabla T$$

Nonzero $L^{\alpha\beta}$:

$$L^{\boldsymbol{m}\boldsymbol{m}} = \frac{\bar{\bar{\Lambda}}}{H_\sigma} = \frac{\bar{\bar{\Lambda}}}{T} \quad \text{and} \quad L^{\sigma\sigma} = \frac{\bar{\kappa}/T}{H_\sigma} = \frac{\bar{\kappa}}{T^2}\,,$$

Note: In $L^{\sigma\sigma} = \bar{\kappa}/T^2$, one T from systematic theory $T := H_\sigma$, while one from phenomenological law: Fourier's heat flux law, $\boldsymbol{q} = \bar{\kappa}\,\nabla T/T$.

4. K-N Metriplectic 4-Brackets for FNS (cont)

K-N Form:

$$M(dF, dG) = F_\sigma G_\sigma \,,$$

$$\Sigma(dF, dG) = \nabla F_{\boldsymbol{m}} : \frac{\bar{\bar{\Lambda}}}{T} : \nabla G_{\boldsymbol{m}} + \nabla F_\sigma \cdot \frac{\bar{\kappa}}{T^2} \cdot \nabla G_\sigma$$

Entropy Production:

$$\dot{S} = (S, H; S, H) = \int_\Omega \Sigma(dH, dH) = \int \nabla \mathbf{v} : \frac{\bar{\bar{\Lambda}}}{T} : \nabla \mathbf{v} + \nabla T \cdot \frac{\bar{\kappa}}{T^2} \cdot \nabla T \geq 0$$

4-bracket:

$$(F, K; G, N) = \int_\Omega \frac{1}{T}\Big[\, [K_\sigma \nabla F_{\mathbf{m}} - F_\sigma \nabla K_{\mathbf{m}}] : \bar{\bar{\Lambda}} : [N_\sigma \nabla G_{\mathbf{m}} - G_\sigma \nabla N_{\mathbf{m}}]$$
$$+ \frac{1}{T}\Big[K_\sigma \nabla F_\sigma - F_\sigma \nabla K_\sigma\Big] \cdot \bar{\kappa} \cdot \Big[N_\sigma \nabla G_\sigma - G_\sigma \nabla N_\sigma\Big]$$

Equations of Motion

Navier-Stokes-Fourier:

$$\partial_t \rho = \{\rho, H\} + (\rho, H; S, H) = -\boldsymbol{v} \cdot \nabla \rho - \rho \nabla \cdot \mathbf{v}$$

$$\partial_t \mathbf{v} = \{\boldsymbol{v}, H\} + (\boldsymbol{v}, H; S, H) = -\boldsymbol{v} \cdot \nabla \boldsymbol{v} - \nabla p/\rho + \frac{1}{\rho} \nabla \cdot (\bar{\bar{\Lambda}} : \nabla \mathbf{v})$$

$$\partial_t \sigma = \{\sigma, H\} + (\sigma, H; S, H) = -\boldsymbol{v} \cdot \nabla \sigma - \sigma \nabla \cdot \mathbf{v}$$
$$+ \nabla \cdot \left(\frac{\bar{\kappa}}{T} \cdot \nabla T \right) + \frac{1}{T^2} \nabla T \cdot \bar{\kappa} \cdot \nabla T + \frac{1}{T} \nabla \mathbf{v} : \bar{\bar{\Lambda}} : \nabla \mathbf{v} \, .$$

Tensors:

$$\Lambda_{ijkl} = \eta \left(\delta_{il}\delta_{jk} + \delta_{jl}\delta_{ik} - \frac{2}{3}\delta_{ij}\delta_{kl} \right) + \zeta \, \delta_{ij}\delta_{kl} \quad \text{and} \quad \kappa_{ij} = \kappa_{ji} \, ,$$

Conclusions

- Reviewed Unified Thermodynamic Algorithm (UTA).

- Produced a general thermodynamically consistent FNS system.

$$\dot{S} = (S, H; S, H) = K(S, H) \quad \leftarrow \textbf{sectional curvature}$$

- Easy to project onto finite element basis and obtain thermodynamically consistent semi-discrete (ODE) form. Didn't discuss.

Future Work?

- Apply algorithm to some plasma problem? Pellet injection, multi collisional species, comet tails, dusty plasmas, etc.?