

# Using the Metriplectic 4-Bracket for Constructing Thermodynamically Consistent Models and Structure Preserving Numerical Algorithms

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**Metriplectic 4-Bracket:** undergrad, **Michael Updike** (geometry), now Princeton grad student, grad student intern, **Azeddine Zaidni** (UTA), UM6, Marrakesh-Safi, Morocco; **Naoki Sato** (collision operators), NIFS, Nagoya, Japan, **William Barham** (numerics), UT Austin.

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## Recent Papers

- A. Zaidni and P. J. Morrison, “[Metriplectic 4-Bracket Algorithm for Constructing Thermodynamically Consistent Dynamical Systems](#),” arXiv:2501.00159v1 [physics.flu-dyn] 30 Dec 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 Non-canonical 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).

## Thermodynamic Consistency – Examples

Navier-Stokes (**inconsistent**):

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

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

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

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

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

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

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

## Thermodynamic Consistency and the UTA

The **dynamical** realization of the first and second laws of thermodynamics: energy conservation and entropy production,

$$\dot{H} = 0 \quad \text{and} \quad \dot{S} \geq 0$$

Recall, thermodynamics has no real dynamics – only vague statements like adiabatic compression or or isothermal expansion, etc.

Here we present **Unified Thermodynamic Algorithm** (UTA) for construction. Important **by-product** re ‘Force-Flux’ relations of nonequilibrium thermodynamics:

$$\mathbf{J}^\alpha = L^{\alpha\beta} \mathbf{X}_\beta \quad \rightarrow \quad \mathbf{J}^\alpha = -L^{\alpha\beta} \nabla(\delta H / \delta \xi^\beta)$$

‘Forces’:  $\mathbf{X} \sim \nabla T, \nabla p, \nabla \mathbf{v}$  etc., UTA removes ambiguous selection.  $L^{\alpha\beta}$  phenomenological coefficients,  $\xi^\beta$  dynamical variables.

# What is Dissipation?

- Not all conservative systems are Hamiltonian
- Not all Hamiltonian systems are conservative
- Not all reversible systems are Hamiltonian
- All finite dynamical systems (autonomous ODEs) are reversible
- Some infinite systems (PDEs) are reversible and some irreversible
- Not all Hamiltonian systems have time reversal symmetry
- Not all systems with time reversal symmetry are Hamiltonian
- $\exists$  systems with time reversible symmetry and global asymptotic stability

## **Dissipation:**

Systems with an increasing entropy and global asymptotic stability have dissipation.

Such systems have a 'vector field' that naturally splits in Hamiltonian and dissipative parts. Hamiltonian is an unambiguous way to define nondissipative. The Metriplectic 4-bracket is an unambiguous way to define dissipative. Together they provide thermodynamic consistency.

# Metriplectic Dynamics

(Metric  $\cup$  Symplectic Flows)

Dynamical System:

$$\dot{O} = \{O, H\} + (O, H; S, H) \quad \leftarrow \text{Poisson} + 4 - \text{bracket}$$

- $O$  any observable (functional of dynamical variables)
- Can be finite or infinite. We will not distinguish much.

# Hamiltonian Review

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

# Noncanonical 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! They can be entropies.).

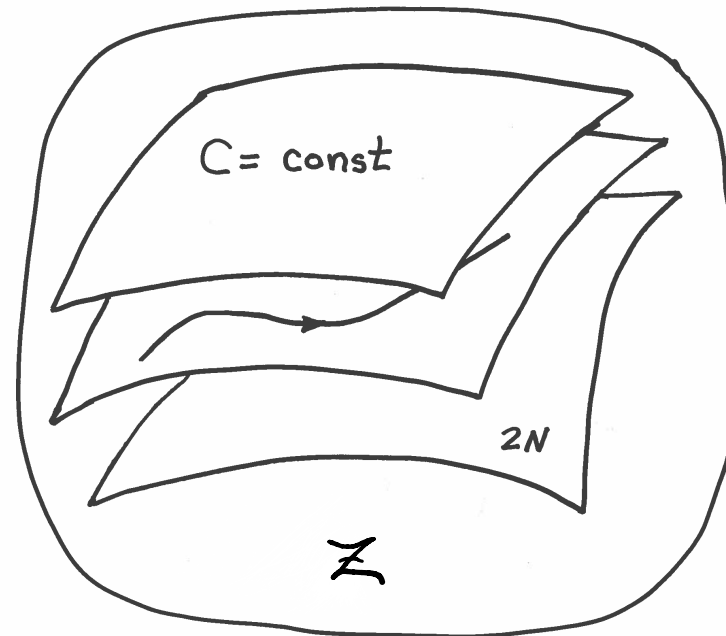


## Poisson Manifold (phase space) $\mathcal{Z}$ Cartoon

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 early ideas: Two important functions  $H$  and  $S$ , symmetries, curvature idea, multilinear brackets.
- Metriplectic manifolds have both Poisson tensor,  $J^{ij}$ , and compatible quadravector  $R^{ijkl}$ , where  $S$  (Casimir) 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 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.**

## Properties – Existence – General Construction Methods

- Thermodynamic Consistency:

$$\dot{H} = \{H, H\} + (H, H; S, H) = 0 \quad \text{and} \quad \dot{S} = (S, H; S, H) \geq 0$$

- 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.

- 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  $\sigma = dS$  and  $\eta = dH$ .

- Methods of construction? We describe two: **Kulkarni-Nomizu and Lie algebra based**. Goal is to develop intuition like building Lagrangians.  $K(\sigma, \eta) \geq 0$  automatic for K-N!

## Construction via Kulkarni-Nomizu Product

Given  $\sigma$  and  $\mu$ , 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:

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

Infinite dimensions:  $\mu \rightarrow M$ ,  $\sigma \rightarrow \Sigma$ .

# 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  $c_s^{kl}$ :

$$(f, k; g, n) = c_r^{ij} c_s^{kl} g^{rs} \frac{\partial f}{\partial z^i} \frac{\partial k}{\partial z^j} \frac{\partial g}{\partial z^k} \frac{\partial n}{\partial z^l}.$$

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  $g_{CK}^{rs} = c_k^{rl} c_l^{sk}$  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.

## Unified Thermodynamic Algorithm (UTA)

UTA is an algorithm for constructing metriplectic systems! Applied to many systems. **So far UTA either reproduces, corrects, or extends for every case considered!**

- Cahn-Hilliard-Navier-Stokes: agrees with Anderson et al.; corrects Guo and Lin
- Brenner-Navier-Stokes: UTA produces Brenner's equations, plus corrects statements, e.g., that the results are most general.
- Generalization of Brenner-Navier-Stokes: UTA produces equations of Reddy et al. (2019). All are generalizations of Navier-Stokes-Fourier with modified dissipation.
- Collisions on noncanonical phase space: Generalization of Landau for drift kinetic, ...

## 4 Steps of the UTA

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

$$\xi = (m = \rho v, \rho, \sigma = \rho s)$$

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

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

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:

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

**Result automatically Thermodynamically consistent!**

### 3. For NSF Ideal Fluid Poisson Bracket Dynamics (pjm-Greene (1980))

Hamiltonian:

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

M-G Poisson Bracket:

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

Equations of Motion:

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

Casimir:

$$S = \int_{\Omega} \rho s = \int_{\Omega} \sigma.$$

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

## 4. Metriplectic 4-Bracket

Old method: guess  $M$  and  $\Sigma$ .

## New Method

Theorem: Order dynamical variables st

$$\begin{aligned}\partial_t \xi^\alpha &= \{\xi^\alpha, H\} + \nabla \cdot \mathbf{J}^\alpha, & \alpha = 1, \dots, N-1, \\ \partial_t \xi^N &= \{\xi^N, H\} + \nabla \cdot \mathbf{J}^N + \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta.\end{aligned}$$

where  $\xi^N = \sigma$ , the entropy density. Above splits Hamiltonian and conservative.

Then

$$\dot{S} = \int_{\Omega} \mathbf{Z}_\alpha \cdot \tilde{L}^{\alpha\beta} \cdot \mathbf{Z}_\beta =: \int_{\Omega} \dot{s}^{prod} \geq 0.$$

and  $\dot{H} \Rightarrow$

$$\mathbf{Z}_\alpha = \nabla H_{\xi^\alpha}, \quad \mathbf{J}^\alpha = -H_{\xi^N} \tilde{L}^{\alpha\beta} \nabla H_{\xi^\beta} = -L^{\alpha\beta} \nabla H_{\xi^\beta}.$$

which leads naturally to

$$M(dF, dG) = F_{\xi^N} G_{\xi^N}, \quad \Sigma(dF, dG) = \nabla(F_{\xi^\alpha}) \frac{L^{\alpha\beta}}{H_{\xi^N}} \nabla(G_{\xi^\beta}).$$

## 4. Metriplectic 4-Bracket General and NSF

General flux expressions:

$$\begin{aligned}\mathbf{J}_\rho &= -L^{\rho\rho} \cdot \nabla H_\rho - L^{\rho m} : \nabla H_m - L^{\rho\sigma} \cdot \nabla H_\sigma, \\ \bar{\mathbf{J}}_m &= -L^{m\rho} \otimes \nabla H_\rho - L^{mm} : \nabla H_m - L^{m\sigma} \otimes \nabla H_\sigma, \\ \mathbf{J}_\sigma &= -L^{\sigma\rho} \cdot \nabla H_\rho - L^{\sigma m} : \nabla H_m - L^{\sigma\sigma} \cdot \nabla H_\sigma,\end{aligned}$$

where  $\mathbf{J}_\rho$  is mass flux,  $\bar{\mathbf{J}}_m$  is momentum flux 2-tensor, and  $\mathbf{J}_\sigma$  is entropy flux.

For **NSF** all zero except:

$$L^{mm} = \bar{\bar{\Lambda}} \quad \text{and} \quad L^{\sigma\sigma} = \frac{\bar{\kappa}}{T}.$$

$\bar{\bar{\Lambda}}$  isotropic 4-tensor,  $\bar{\kappa}$  conduction 2-tensor

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

Note in  $\bar{\kappa}/T^2$  one  $T$  from  $H$  one from  $L^{\alpha\beta}$ .  $\Sigma$  sectional curvature density?

## 4. Metriplectic 4-Bracket for NSF Generalizations

For **BNSF** all zero except:

$$\begin{aligned} L^{m\rho} &= \tilde{D}_\rho \mathbf{m}, & L^{m\sigma} &= \tilde{D}\hat{\sigma} \mathbf{m}, & L^{mm} &= \bar{\Lambda} + \tilde{D} \mathbf{m} \otimes \bar{I} \otimes \mathbf{m}. \\ L^{\sigma\rho} &= \tilde{D}_\rho \hat{\sigma} \bar{I}, & L^{\sigma\sigma} &= \frac{\bar{\kappa}}{T} + \tilde{D}\hat{\sigma}^2 \bar{I} & L^{\sigma m} &= \tilde{D}\hat{\sigma} \bar{I} \otimes \mathbf{m} \end{aligned}$$

$$\dot{S} = \int_{\Omega} \frac{1}{T} \left[ \frac{\tilde{D}}{\kappa_T^2 \rho^2} |\nabla \rho|^2 + \nabla T \cdot \frac{\bar{\kappa}}{T} \cdot \nabla T + \nabla \mathbf{v} : \bar{\Lambda} : \nabla \mathbf{v} \right] \geq 0.$$

Similarly, the generalization of Reddy et al. (2019) falls out. It can be further generalized.



## Final Comments

- UTA based on the metriplectic 4-bracket, a proven framework, provides a direct method for constructing thermodynamically consistent systems.
- Metriplectic 4-brackets are easy to discretize while maintaining symmetries. First numerical implementation via 4-bracket discretization (Barham et al. 2024) 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  $\rho(x, t)$

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

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