Thermodynamically consistent 2-phase flow via metriplectic 4-bracket dynamics

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- Theory of thermodynamically consistent theories.
- An algorithm for constructing such theories.
- Use algorithm to construct consistent theories for 2-phase flow.
Old and New

Old:

New:
Thermodynamic Consistency – Examples

Navier-Stokes (inconsistent):

\[
\begin{align*}
\partial_t v &= -v \cdot \nabla v - \frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot \mathcal{T} \quad \leftarrow \mathcal{T} \text{ viscous stress tensor } \sim \nabla v \\
\partial_t \rho &= -\nabla \cdot (\rho v)
\end{align*}
\]

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

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

\[
\begin{align*}
\partial_t v &= -v \cdot \nabla v - \frac{1}{\rho} \nabla p + \frac{1}{\rho} \nabla \cdot \mathcal{T} \\
\partial_t \rho &= -\nabla \cdot (\rho v) \\
\partial_t s &= -v \cdot \nabla s - \frac{1}{\rho T} \nabla \cdot \mathbf{q} + \frac{1}{\rho T} \mathcal{T} : \nabla v \quad \text{heat flux & viscous heating}
\end{align*}
\]

\[H = \int_\Omega \rho |v|^2/2 + \rho u(\rho, s), \quad \dot{H} = 0 \quad \text{and} \quad S = \int_\Omega \rho s \rightarrow \dot{S} \geq 0\]
\[ S_0 > S_1 \]
\[ S_0 > S_0 \]
\[ S = K(s, H) \]
\[ = (s, H, s, H) \geq 0 \]
Cahn-Hilliard Equation (1958)

Equation of Motion:

\[
\frac{\partial c}{\partial t} = \nabla^2 \left( c^3 - c - \nabla^2 c \right) = \nabla^2 \delta F \delta c,
\]

for concentration \( c \).

“Free Energy”:

\[
F = \int d^3x \left( \frac{c^4}{4} - \frac{c^2}{2} + |\nabla c|^2 \right) \equiv H - TS.
\]

A phase separation (diffuse interface) solution:
Goal

Construct:

• Cahn-Hilliard $\cup$ Navier-Stokes $=\,$ Cahn-Hilliard - Navier-Stokes (CHNS)

• Thermodynamically consistent with complete set of fluxes and affinities.
**All 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, $V_D$: not conservative of something, relaxation/asymptotic stability, etc.

**General Hamiltonian Form:**

For finite dimension:

\[ V_H = J \frac{\partial H}{\partial z} = \{z, H\} \quad \text{or} \quad V_H = J \frac{\delta H}{\delta \psi} \]

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

**General Dissipation:**

\[ V_D = ? \ldots \quad \rightarrow \quad V_D = G \frac{\partial S}{\partial z} \]

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

Identify configuration space:

- Coordinates $q \in Q$.
- 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.
Metriplectic Algorithm - 4 Steps

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

$$\Psi = \{v, \rho, s, c\} \quad \text{or} \quad \Psi = \{m = \rho v, \rho, \sigma = \rho s, \bar{c} = \rho c\}$$

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

$$H^a = \int_{\Omega} \frac{\rho}{2}|v|^2 + \rho u(\rho, s, c) + \frac{\rho^a}{2}\lambda u \Gamma^2(\nabla c) \quad \text{and} \quad S^a = \int_{\Omega} \rho s + \frac{\rho^a}{2}\lambda s \Gamma^2(\nabla c)$$

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

4. Construct metriplectic 4-bracket $(F, K; G, N)$ via Kulkarni-Nomizu product to obtain EoMs:

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

Result automatically Thermodynamically consistent!

* Here $a \in \{0, 1\}$ is a parameter; $\Gamma$ Euler homogenous deg 1 (Taylor 1992 weighted mean curvature surface effects); when $\Gamma^2(\nabla c) = |\nabla c|^2$, cf. $F = H - TS$ of C-H.
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:

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

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

\[
\dot{z}^i = J_{c}^{ij} \frac{\partial H}{\partial z^j} = \{z^i, H\}_c, \quad J_c = \begin{pmatrix} 0_N & I_N \\ -I_N & 0_N \end{pmatrix},
\]

\(J_c := \text{Poisson tensor}, \text{ Hamiltonian bi-vector, cosymplectic form} \)
Noncanonical Hamiltonian Structure

Sophus Lie (1890) → PJM (1980) → Poisson Manifolds etc.

Noncanonical Coordinates:
\[ \dot{z}^a = \{z^a, H\} = J^{ab}(z) \frac{\partial H}{\partial z^b}, \quad a, b = 1, 2, \ldots M \]

Noncanonical Poisson Bracket:
\[ \{f, g\} = \frac{\partial f}{\partial z^a} J^{ab}(z) \frac{\partial g}{\partial z^b}, \quad J(z) \neq J_c \]

Poisson Bracket Properties:
- antisymmetry \( \rightarrow \{f, g\} = -\{g, f\} \)
- Jacobi identity \( \rightarrow \{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0 \)
- Leibniz \( \rightarrow \{fh, g\} = f\{h, g\} + \{h, g\}f \)

Jean Gaston Darboux: \( detJ \neq 0 \Rightarrow J \rightarrow J_c \) Canonical Coordinates

Sophus Lie: \( detJ = 0 \Rightarrow \) Canonical Coordinates plus Casimirs (Lie’s distinguished functions!)
Poisson Brackets – Flows on Poisson Manifolds

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

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

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

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

Geometrically \( \mathcal{C}^\infty(\mathcal{Z}) \equiv \Lambda^0(\mathcal{Z}) \) 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.,

\[
\dot{z}^a = J^{ab}(z) \frac{\partial H(z)}{\partial z^b}, \quad \mathcal{Z}'s \: \text{coordinate patch } z = (z^1, \ldots, z^M)
\]

Because of degeneracy, \( \exists \) functions \( C \) s.t. \( \{ f, C \} = 0 \) for all \( f \in \mathcal{C}^\infty(\mathcal{Z}) \). Casimir invariants.
Poisson Manifold (phase space) $\mathcal{Z}$ Cartoon

Degeneracy in $J \Rightarrow$ Casimirs:

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

Lie-Darboux Foliation by Casimir (symplectic) leaves:
3. Gibbs-Euler Poisson Bracket Dynamics

Hamiltonian:
\[ H = \int_{\Omega} \frac{\rho|v|^2}{2} + \rho u(\rho, s, c) , \quad T = \frac{\partial u}{\partial s} , \quad p = \rho^2 \frac{\partial u}{\partial \rho} , \quad \mu = \frac{\partial u}{\partial c} . \]

Poisson Bracket:
\[ \{F, G\} = -\int_{\Omega} m \cdot [F_m \cdot \nabla G_m - G_m \cdot \nabla F_m] + \rho [F_m \cdot \nabla G_{\rho} - G_m \cdot \nabla F_{\rho}] \]
\[ + \sigma [F_m \cdot \nabla G_{\sigma} - G_m \cdot \nabla F_{\sigma}] + \tilde{c} [F_m \cdot \nabla G_{\tilde{c}} - G_m \cdot \nabla F_{\tilde{c}}] . \]

Equations of Motion:
\[ \partial_t v = \{v, H\} = -v \cdot \nabla v - \nabla p/\rho , \quad \partial_t \rho = \{\rho, H\} = -\nabla \cdot (\rho v) , \]
\[ \partial_t \tilde{c} = \{\tilde{c}, H\} = -\nabla \cdot (\tilde{c} v) , \quad \partial_t \sigma = \{\sigma, H\} = -\nabla \cdot (\sigma v) \]

Casimir:
\[ S = \int_{\Omega} \rho s \neq S^a ! \]

Coordinate Change:
\[ \rho s^a = \rho s + \rho^a \lambda_s \Gamma^2(\nabla c) , \quad m, \rho, c \quad \text{unchanged} . \]

Note \( F_m = \delta F/\delta m \), etc., functional derivatives.
Metriplectic 4-Bracket: \((f, k; g, n)\)

**Metriplectic Dynamics:**

\[
\dot{o} = \{o, H\} + (o, H; S, H)
\]
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, $\mathcal{F} = H - TS$, 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):

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

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:

\[(f, k; g, n) = R^{ijkl}(z) \frac{\partial f}{\partial z^i} \frac{\partial k}{\partial z^j} \frac{\partial g}{\partial z^k} \frac{\partial n}{\partial z^l}.\]

\(\leftarrow\) 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 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? We describe two: Kulkarni-Nomizu and Lie algebra based. Goal is to develop intuition like building Lagrangians.
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

\[
\sigma \otimes \mu (df, dk, dg, dn) = \sigma (df, dg) \mu (dk, dn) - \sigma (df, dn) \mu (dk, dg) + \mu (df, dg) \sigma (dk, dn) - \mu (df, dn) \sigma (dk, dg).
\]

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: Denoted $\mathfrak{g}$, is a vector space (over $\mathbb{R}$, $\mathbb{C}$, for us $\mathbb{R}$) with binary, bilinear product $[\cdot,\cdot]: \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$. 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 $A \times (B \times C) + B \times (C \times A) + C \times (A \times B) \equiv 0$.

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

$$\{f, g\} = \langle z, [\nabla f, \nabla g] \rangle = \frac{\partial f}{\partial z_i} c_{ij}^k z_k \frac{\partial g}{\partial z_j}, \quad i,j,k = 1, 2, \ldots, \dim \mathfrak{g}$$

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

• Covariant connection $\nabla: \mathfrak{X} \times \mathfrak{X} \to \mathfrak{X}$. A contravariant connection $D: \Lambda^{1}(Z) \times \Lambda^{1}(Z) \to \Lambda^{1}(Z)$ satisfying Koszul identities, but Leibniz becomes $D_{\alpha}(f \gamma) = f D_{\alpha} \gamma + J(\alpha)[f] \gamma$ where $J(\alpha)[f] = \alpha_{i} J^{ij} \partial f / \partial z^{j}$ is a 0-form that replaces the term $X(f)$ (Fernandes, 2000). Here $\alpha, \beta, \gamma \in \Lambda^{1}(Z)$, $f \in \Lambda^{0}(Z)$. Add a metric, build 4-bracket like curvature from connection.
4. K-N Metriplectic 4-Brackets for CHNS

**K-N Form:**

\[
\begin{align*}
M(dF, dG) &= F_{\sigma a} G_{\sigma a}, \\
\Sigma(dF, dG) &= \nabla F_m : \bar{\Lambda}_1 : \nabla G_m + \nabla F_{\sigma a} : \bar{\Lambda}_2 : \nabla G_{\sigma a} + \nabla \mathcal{L}_c^{a}(F) : \bar{\Lambda}_3 : \mathcal{L}_c^{a}(G),
\end{align*}
\]

with pseudodifferential operator \( \mathcal{L}_c^{a}F := \nabla \left( F_{\tilde{c}} + \nabla \cdot \left( \rho^a \lambda_3 \Gamma \xi F_{\sigma a} \right) / \rho \right). \)

**4-bracket:**

\[
(F, K; G, N)^a = \frac{1}{\Omega T} \int \left[ [K_{\sigma a} \nabla F_m - F_{\sigma a} \nabla K_m] : \bar{\Lambda} : [N_{\sigma a} \nabla G_m - G_{\sigma a} \nabla N_m] \\
+ \frac{1}{T} [K_{\sigma a} \nabla F_{\sigma a} - F_{\sigma a} \nabla K_{\sigma a}] \cdot \bar{\kappa} \cdot \left[ N_{\sigma a} \nabla G_{\sigma a} - G_{\sigma a} \nabla N_{\sigma a} \right] \\
+ \left[ K_{\sigma a} \mathcal{L}_c^{a}(F) - F_{\sigma a} \mathcal{L}_c^{a}(K) \right] \cdot \bar{D} \cdot \left[ N_{\sigma a} \mathcal{L}_c^{a}(G) - G_{\sigma a} \mathcal{L}_c^{a}(N) \right] \right].
\]
Equations of Motion - Case $a = 1, \Gamma = |\nabla c|$

CHNS system for $a = 1$:

$$
\partial_t v = \{v, H^1\}^1 + (v, H^1; S^1, H^1)^1 = -v \cdot \nabla v - \frac{1}{\rho} \nabla \cdot \left[ pI + \lambda f \rho \Gamma \xi \otimes \nabla c \right] + \frac{1}{\rho} \nabla \cdot (\bar{\Lambda} : \nabla v),
$$

$$
\partial_t \rho = \{\rho, H^1\}^1 + (\rho, H^1; S^1, H^1)^1 = -\nabla \cdot (\rho v),
$$

$$
\partial_t \tilde{c} = \{\tilde{c}, H^1\}^1 + (\tilde{c}, H^1; S^1, H^1)^1 = -\nabla \cdot (\tilde{c} v) + \nabla \cdot (\bar{D} \cdot \nabla \mu^1_1),
$$

$$
\partial_t \sigma^1_{\text{Total}} = \{\sigma^1_{\text{Total}}, H^1\}^1 + (\sigma^1_{\text{Total}}, H^1; S^1, H^1)^1 = -\nabla \cdot (\sigma^1_{\text{Total}} v) + \nabla \cdot \left( \frac{\bar{\kappa}}{T} \cdot \nabla T \right) + \frac{1}{T^2} \nabla T \cdot \bar{\kappa} \cdot \nabla T
$$

$$
+ \frac{1}{T} \nabla v : \bar{\Lambda} : \nabla v + \frac{1}{T} \nabla \mu^1_1 \cdot \bar{D} \cdot \nabla \mu^1_1.
$$

Special case has $H$ and $S$ same as Guo and Lin, JFM (2015). But EoMs do **not** agree!
Ours generalizes theirs and conserves energy, theirs does **not**!
Equations of Motion - Case $a = 0, \Gamma$ general

CHNS for $a = 0$:

$$
\begin{align*}
\partial_t v &= \{v, H^0\}^0 + (v, H^0; S^0, H^0)^0 \\
&= -v \cdot \nabla v - \frac{1}{\rho} \nabla \cdot \left[ (p - \lambda f \Gamma^2/2) I + \lambda f \Gamma \xi \otimes \nabla c \right] + \frac{1}{\rho} \nabla \cdot (\bar{\Lambda} : \nabla v), \\
\partial_t \rho &= \{\rho, H^0\}^0 + (\rho, H^0; S^0, H^0)^0 = -\nabla \cdot (\rho v) \\
\partial_t \bar{c} &= \{\bar{c}, H^0\}^0 + (\bar{c}, H^0; S^0, H^0)^0 = -\nabla \cdot (\bar{c} v) + \nabla \cdot (\bar{D} \cdot \nabla \mu_0^T), \\
\partial_t \sigma^0_{\text{Total}} &= \{\sigma^0_{\text{Total}}, H^0\}^0 + (\sigma^0_{\text{Total}}, H^0; S^0, H^0)^0 \\
&= -\nabla \cdot (\sigma^0_{\text{Total}} v) + \nabla \cdot \left( \frac{\bar{k}}{T} \cdot \nabla T \right) + \frac{1}{T^2} \nabla T \cdot \bar{k} \cdot \nabla T \\
&\quad + \frac{1}{T} \nabla v : \bar{\Lambda} : \nabla v + \frac{1}{T} \nabla \mu_0^T \cdot \bar{D} \cdot \nabla \mu_0^T.
\end{align*}
$$

Conclusions

• Produced a general thermodynamically consistent CHNS system.

\[ \dot{S}^a = (S^a, H^a; S^a, H^a)^a = K(S^a, H^a) \leftarrow \text{sectional curvature} \]

\[ = \int_\Omega \frac{1}{T} \left[ \nabla \cdot \tilde{\kappa} \cdot \nabla + \frac{1}{T} \nabla T \cdot \tilde{\kappa} \cdot \nabla T + \nabla \mu^a_{\Gamma} \cdot \tilde{D} \cdot \nabla \mu^a_{\Gamma} \right] \geq 0. \]

• General system reduces to two thermodynamically consistent CHNS systems: Anderson et al. yes, while Guo and Lin, almost.

Future Work?

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