Variational-metriplectic formulations of compressible, multiphase, multicomponent geophysical fluids

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What are Lagrangian and Hamiltonian formulations?

In classical mechanics, there are three (equivalent) ways of expressing dynamics, or *formulations*:

1. Newtonian Formulation: Force Balances

$$\mathbf{F} = m\mathbf{a}$$

2. Lagrangian (Variational) Formulation: Lagrangian $\mathcal{L}$ and Variational Principle, canonical (Hamilton's principle, Lagrangian coordinates), non-canonical (Eulerian coordinates, Euler-Poincare)

$$\delta \int_0^T L(q_i, \dot{q}_i) dt = 0$$

3. Hamiltonian Formulation: Hamiltonian H and Poisson Brackets/Structure $\{\mathrm{A}, \mathrm{B}\}$, canonical ($q_i$, $p_i = \frac{\delta \mathcal{L}}{\delta \dot{q}_i}$, Lagrangian coordinates) non-canonical (Lie-Poisson or curl-form, semi-direct product), Legendre transform (may not exist!)

$$\frac{\mathrm{d}\mathrm{F}}{\mathrm{d}t} = \{\mathrm{F}, \mathrm{H}\} = \sum_i \frac{\partial F}{\partial q_i} \cdot \frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i} \cdot \frac{\partial H}{\partial q_i}$$

Why use Lagrangian and Hamiltonian formulations?

Lagrangian and Hamiltonian formulations have proven useful (amongst other things) for

1. Understanding conservation laws and circulation theorems
2. Inclusion of constraints such as semi-compressibility
3. Development of structure-preserving numerical schemes
4. Systematic derivation of consistent new models and approximations
5. Energy-Casimir theory: Pseudo-energy/momentum, finite amplitude invariants, wave-activity conservation laws

However, until recently, restricted to reversible dynamics

Key Question: how can we extend these formulations to irreversible dynamics, such that

–Consistent treatment of irreversible processes, in terms of the 1st and 2nd laws of thermodynamics

–Recovers the standard approach in absence of irreversible processes

Assumptions, Domain and Variables

Fully compressible, multicomponent, multiphase fluid

1. Predicted variables: n component densities ρ_i, entropy density s, relative velocity $\mathbf{u}$ (Lagrangian formulation), absolute momentum $\mathbf{m}$ (Lie-Poisson Hamiltonian formulation)
2. General domain $\Omega \subset \mathbb{M}$, with associated rotational velocity $\mathbf{R}$ and geopotential Φ, arbitrary equation of state
3. Can get standard geophysical approximations (shallow, traditional, spherical) by approximating $\mathbf{R}$, Φ and $\mathbb{M}$

Key Assumptions

1. Single velocity $\mathbf{u}$ and temperature T for all components
2. Closed boundaries: $\mathbf{u} \cdot \hat{\mathbf{n}} = 0$ on $\partial\Omega$

Alternative predicted variables: total density $\rho = \sum_{i=1}^{n} \rho_i$, specific concentrations $q_i = \frac{\rho_i}{\rho}$, specific entropy $\eta = \frac{s}{\rho}$, absolute velocity $\mathbf{v}$ (leads to curl-form Hamiltonian and metriplectic formulations, not discussed further)

Reversible Dynamics: Lagrangian Formulation

Variational Principle: Given *Lagrangian* $\mathcal{L}[\mathbf{u}, \rho_i, s]$, take variations

$$\delta \int_0^T \mathcal{L}[\mathbf{u}, \rho_i, s] dt = 0,$$

where variations $\delta\,\mathbf{u}$, $\delta\rho_i$ and δs are given by

$$\delta\,\mathbf{u} = \partial_t \boldsymbol{\zeta} + \mathbf{u} \cdot \nabla \boldsymbol{\zeta} - \boldsymbol{\zeta} \cdot \nabla \mathbf{u} \quad \delta\rho_i = -\nabla \cdot (\rho_i\, \boldsymbol{\zeta}) \quad \delta s = -\nabla \cdot (s\, \boldsymbol{\zeta})$$

with $\boldsymbol{\zeta} \cdot \hat{\mathbf{n}} = 0$ on $\partial\Omega$ and $\boldsymbol{\zeta} = 0$ for $t = 0, T$. Produces the *Euler-Lagrange* equations

$$\partial_t \frac{\delta \mathcal{L}}{\delta \mathbf{u}} + \pounds_{\mathbf{u}} \frac{\delta \mathcal{L}}{\delta \mathbf{u}} - \sum_i \rho_i \nabla \frac{\delta \mathcal{L}}{\delta \rho_i} - s \nabla \frac{\delta \mathcal{L}}{\delta s} = 0$$

which are supplemented with *kinematic* equations

$$\partial_t \rho_i + \nabla \cdot (\rho_i\, \mathbf{u}) = 0 \qquad \partial_t s + \nabla \cdot (s\, \mathbf{u}) = 0$$

The *Lie derivative* is $\pounds_{\mathbf{u}} \mathbf{m} = (\nabla \times \mathbf{m}) \times \mathbf{u} + \nabla(\mathbf{u} \cdot \mathbf{m}) + \mathbf{m}\, \mathrm{div}\, \mathbf{u}$

Reversible Dynamics: Hamiltonian Formulation (I)

Get the *Hamiltonian* $\mathsf{H}[\mathbf{m}, \rho_i, s]$ using a *Legendre transform*:

$$\mathsf{H}[\mathbf{m}, \rho_i, s] = \int_\Omega \mathbf{u} \cdot \mathbf{m} \, \mathrm{d}x - \mathcal{L}[\mathbf{u}, \rho_i, s],$$

where $\mathbf{m} := \frac{\delta \mathcal{L}}{\delta \mathbf{u}}$, where $\mathsf{H}[\mathbf{m}, \rho_i, s]$ has functional derivatives

$$\frac{\delta \mathsf{H}}{\delta \mathbf{m}} := \mathbf{F}^m = \mathbf{u} \qquad \frac{\delta \mathsf{H}}{\delta \rho_i} := B_i^m = -\frac{\delta \mathcal{L}}{\delta \rho_i} \qquad \frac{\delta \mathsf{H}}{\delta s} := T^m = -\frac{\delta \mathcal{L}}{\delta s}$$

The evolution of an arbitrary functional $\mathsf{F}[\mathbf{m}, \rho_i, s]$ is governed by

$$\frac{\mathrm{d}\mathsf{F}}{\mathrm{d}t} = \{\mathsf{F}, \mathsf{H}\}$$

where the *Lie-Poisson* bracket $\{\mathsf{A}, \mathsf{B}\}$ is anti-symmetric, bilinear, and satisfies the Leibniz rule and the Jacobi identity:

$$\{\mathsf{A}, \mathsf{B}\} = -\int_\Omega \mathbf{m} \cdot \left[\frac{\delta \mathsf{A}}{\delta \mathbf{m}} \cdot \nabla \frac{\delta \mathsf{B}}{\delta \mathbf{m}} - \frac{\delta \mathsf{B}}{\delta \mathbf{m}} \cdot \nabla \frac{\delta \mathsf{A}}{\delta \mathbf{m}} \right] \mathrm{d}x$$

$$- \int_\Omega \rho_i \left(\frac{\delta \mathsf{A}}{\delta \mathbf{m}} \cdot \nabla \frac{\delta \mathsf{B}}{\delta \rho_i} - \frac{\delta \mathsf{B}}{\delta \mathbf{m}} \cdot \nabla \frac{\delta \mathsf{A}}{\delta \rho_i} \right) \mathrm{d}x - \int_\Omega s \left(\frac{\delta \mathsf{A}}{\delta \mathbf{m}} \cdot \nabla \frac{\delta \mathsf{B}}{\delta s} - \frac{\delta \mathsf{B}}{\delta \mathbf{m}} \cdot \nabla \frac{\delta \mathsf{A}}{\delta s} \right) \mathrm{d}x$$

Reversible Dynamics: Hamiltonian Formulation (II)

Insert $\frac{\delta H}{\delta x}$ into $\{F, H\}$ to get general *equations of motion*

$$\partial_t \mathbf{m} + \pounds_{\mathbf{u}} \mathbf{m} + s\nabla T^m + \sum_i \rho_i \nabla B_i^m = 0$$

$$\partial_t \rho_i + \nabla \cdot (\rho_i \mathbf{F}^m) = 0 \qquad \partial_t s + \nabla \cdot (s \mathbf{F}^m) = 0$$

Anti-symmetry of $\{A, B\}$ gives *energy conservation*

$$\frac{dH}{dt} = \{H, H\} = -\{H, H\} = 0$$

The Lie-Poisson bracket also has *Casimirs* $C[\mathbf{m}, \rho_i, s]$ that satisfy

$$\{A, C\} = 0 \text{ for all } A \longrightarrow \frac{dC}{dt} = \{C, H\} = 0$$

One example is

$$C_1 = \int_\Omega \rho f(\eta, q_i) \mathrm{d}x$$

where f is an arbitrary function, which has as special cases *total mass* ($f = 1$), *component mass* ($f = q_i$) and *total entropy* ($f = \eta$)

For a fully compressible, multicomponent, multiphase fluid

$$\mathcal{L}[\mathbf{u}, \rho_i, s] = \int_\Omega \rho\,(K + \mathbf{u}\cdot\mathbf{R} - \Phi - U)\,\mathrm{d}x$$

giving absolute momentum $\mathbf{m} = \frac{\delta\mathcal{L}}{\delta\mathbf{u}} = \rho(\mathbf{u} + \mathbf{R})$ and

$$\mathrm{H}[\mathbf{m}, \rho_i, s] = \int_\Omega \rho\,[K + \Phi + U]\,\mathrm{d}x$$

with *internal energy* $U(\alpha, \eta, q_i)$, *kinetic energy* $K = \frac{1}{2\rho^2}|\mathbf{m} - \rho\mathbf{R}|^2$ and *geopotential* $\Phi(\vec{x})$. Functional derivatives are

$$\frac{\delta\mathrm{H}}{\delta\,\mathbf{m}} = \mathbf{u} \quad \frac{\delta\mathrm{H}}{\delta\rho_i} = -K - \mathbf{u}\cdot\mathbf{R} + \Phi + \mu_i \quad \frac{\delta\mathrm{H}}{\delta s} = T$$

with *temperature* $T = \frac{\partial U}{\partial s}$, *chemical potential* $\mu_i = \frac{\partial U}{\partial q_i}$, and therefore specific equations of motion are

$$\partial_t\,\mathbf{m} + \pounds_{\mathbf{u}}\,\mathbf{m} - \rho\nabla(K + \mathbf{u}\cdot\mathbf{R}) + \rho\nabla\Phi + \nabla p = 0$$

$$\partial_t\rho_i + \nabla\cdot(\rho_i\,\mathbf{u}) = 0 \qquad \partial_t s + \nabla\cdot(s\,\mathbf{u}) = 0$$

Irreversible Dynamics: Lagrangian Formulation (I)

Consider a fluid under the irreversible processes of *phase change*, *heat conduction*, *diffusion* and *viscosity*. The variational formulation is

$$\delta \int_0^T \left[\mathcal{L} + \sum_i \rho_i D_t w_i + (s - \sigma) D_t \gamma \right] dt = 0$$

with no-slip boundary conditions $\mathbf{u}\,|_{\partial\Omega} = 0$, and with *phenomenological* and *variational* constraints

$$\frac{\delta \mathcal{L}}{\delta s} \bar{D}_t \sigma = -\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u} + \mathbf{j}_{\mathsf{s}} \cdot \nabla D_t \gamma + \sum_i \mathbf{j}_{\mathsf{i}} \cdot \nabla D_t w_i + j_i D_t w_i$$

$$\frac{\delta \mathcal{L}}{\delta s} \bar{D}_\delta \sigma = -\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \boldsymbol{\zeta} + \mathbf{j}_{\mathsf{s}} \cdot \nabla D_\delta \gamma + \sum_i \mathbf{j}_{\mathsf{i}} \cdot \nabla D_\delta w_i + j_i D_\delta w_i$$

with Lagrangian derivatives $\bar{D}_t x = \partial_t x + \nabla \cdot (\mathbf{u}\, x)$ and $D_t x = \partial_t x + \mathbf{u} \cdot \nabla x$ and variations $\delta\, \mathbf{u} = \partial_t \boldsymbol{\zeta} + \mathbf{u} \cdot \nabla \boldsymbol{\zeta} - \boldsymbol{\zeta} \cdot \nabla \mathbf{u}$, $\delta \rho_i$, δs, δw_i, $\delta \sigma$, $\delta \gamma$ where $\boldsymbol{\zeta} = \delta w_i = \delta \gamma = 0$ for $t = 0, T$ and $\delta \gamma|_{\partial\Omega} = \delta w_i|_{\partial\Omega} = 0$. To pass from the phenomenological to variational constraint, replace time derivatives with delta variations: $\bar{D}_\delta x = \delta x + \nabla \cdot (\boldsymbol{\zeta} x)$ and $D_\delta x = \delta x + \boldsymbol{\zeta} \cdot \nabla x$

The Euler-Lagrange equations are

$$\begin{aligned}
\partial_t \frac{\delta \mathcal{L}}{\delta \mathbf{u}} + \pounds_{\mathbf{u}} \frac{\delta \mathcal{L}}{\delta \mathbf{u}} - \sum_i \rho_i \nabla \frac{\delta \mathcal{L}}{\delta \rho_i} - s \nabla \frac{\delta \mathcal{L}}{\delta s} - \nabla \cdot \boldsymbol{\sigma}^{\mathrm{fr}} &= 0 \\
\partial_t \rho_i + \nabla \cdot (\rho_i \, \mathbf{u}) + \nabla \cdot \mathbf{j}_{\mathrm{i}} - j_i &= 0 \\
\frac{\delta \mathcal{L}}{\delta s} (\bar{D}_t s + \nabla \cdot \mathbf{j}_{\mathrm{s}}) + \boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u} + \mathbf{j}_{\mathrm{s}} \cdot \nabla T + \sum_i (\mathbf{j}_{\mathrm{i}} \cdot \nabla \mu_i + j_i \mu_i) &= 0
\end{aligned}$$

where $\boldsymbol{\sigma}^{\mathrm{fr}}$ is the *viscous stress tensor*, $\mathbf{j}_{\mathrm{i}}$ is the *diffusion flux* for component i, j_i is the *conversion rate* for component i and $\mathbf{j}_{\mathrm{s}}$ is the *entropy flux density*; with boundary conditions $\mathbf{j}_{\mathrm{s}} \cdot \hat{\mathbf{n}} = \mathbf{j}_{\mathrm{i}} \cdot \hat{\mathbf{n}} = 0$ on $\partial\Omega$; and *mass control conditions* $\sum_i \mathbf{j}_{\mathrm{i}} = 0$ and $\sum_i j_i = 0$.

Irreversible Dynamics: Metriplectic Formulation

Now evolution of $F[\mathbf{m}, \rho_i, s]$ is governed by

$$\frac{dF}{dt} = \{F, H\} + (F, S)$$

where the *metric bracket* (F, S) is symmetric, bilinear and satisfies the Leibniz rule; and $S = \int_\Omega s$ is total entropy and a Casimir of the Lie-Poisson bracket. Also have the requirements

$$(H, S) = 0 \qquad (S, S) \geqslant 0$$

The first requirement gives *1st law of thermodynamics* $\frac{dH}{dt} = 0$, and the second gives the *2nd law of thermodynamics* $\frac{dS}{dt} \geqslant 0$

$$\begin{aligned}(A, B) = &\int \frac{\delta A}{\delta s} \operatorname{div} \boldsymbol{\sigma}^{\mathrm{fr}} \cdot \frac{\delta B}{\delta \mathbf{m}} + \int \frac{\delta B}{\delta s} \operatorname{div} \boldsymbol{\sigma}^{\mathrm{fr}} \cdot \frac{\delta A}{\delta \mathbf{m}} + \int \frac{1}{T} \frac{\delta A}{\delta s} \frac{\delta B}{\delta s} \left(\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u} - \operatorname{div}(T\, \mathbf{j}_{\mathrm{s}}) \right) \\ &+ \sum_i \int \frac{\delta A}{\delta s} (-\operatorname{div} \mathbf{j}_{\mathrm{i}} + j_i) \frac{\delta B}{\delta \rho_i} + \sum_i \int \frac{\delta B}{\delta s} (-\operatorname{div} \mathbf{j}_{\mathrm{i}} + j_i) \frac{\delta A}{\delta \rho_i} \\ &+ \sum_i \int \frac{1}{T} \frac{\delta A}{\delta s} \left(-\mathbf{j}_{\mathrm{i}} \cdot \nabla \mu_i - j_i \mu_i \right) \frac{\delta B}{\delta s}\end{aligned}$$

One of several possible brackets that all give the correct equations of motion and entropy generation rate. Not quite metriplectic, would need $(H, A) = 0$

Irreversible Dynamics: Equations of Motion

Now inserting $\frac{\delta \mathsf{H}}{\delta x}$ into the Lie-Poisson bracket and $\frac{\delta \mathsf{S}}{\delta x}$ into the metric bracket, where

$$\frac{\delta\, \mathsf{S}}{\delta\, \mathbf{m}} = 0 \qquad \frac{\delta\, \mathsf{S}}{\delta \rho_i} = 0 \qquad \frac{\delta\, \mathsf{S}}{\delta s} = 1$$

gives the equations of motion

$$\begin{aligned} \partial_t\, \mathbf{m} + \cdots - \nabla \cdot \boldsymbol{\sigma}^{\mathrm{fr}} &= 0 \\ \partial_t \rho_i + \cdots + \nabla \cdot \mathbf{j}_{\mathrm{i}} - j_i &= 0 \\ \partial_t s + \cdots + \nabla \cdot \mathbf{j}_{\mathrm{s}} - \frac{1}{T}\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u} + \frac{1}{T}\mathbf{j}_{\mathrm{s}} \cdot \nabla T + \frac{1}{T}\sum_i (\mathbf{j}_{\mathrm{i}} \cdot \nabla \mu_i + j_i \mu_i) &= 0 \end{aligned}$$

It remains to *parameterize* the *thermodynamic fluxes* $(\boldsymbol{\sigma}^{\mathrm{fr}}, \mathbf{j}_{\mathrm{i}}, j_i, \mathbf{j}_{\mathrm{s}})$ in terms of the *thermodynamic forces* (Def $\mathbf{u} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u})$, ∇T, $\nabla \mu_i$, μ_i) to close system, such that the *entropy generation* $(\mathsf{S}, \mathsf{S}) \geqslant 0$ is positive-definite

The *entropy generation rate* I is given by $(S, S) = \int I$ as

$$TI = J_\alpha X_\alpha = \left(\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u}\right) - \mathbf{j}_{\mathsf{s}} \cdot \nabla T + \sum_i (-\mathbf{j}_{\mathsf{i}} \cdot \nabla \mu_i - j_i \mu_i)$$

where $J_\alpha = (\boldsymbol{\sigma}^{\mathrm{fr}}, \mathbf{j}_{\mathsf{i}}, j_i, \mathbf{j}_{\mathsf{s}})$ denotes the *thermodynamic fluxes* and $X_\alpha = (\mathrm{Def}\ \mathbf{u} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^T \mathbf{u}), \nabla T, \nabla \mu_i, \mu_i)$ the *thermodynamic forces*. Assume a linear relationship between forces and fluxes

$$J_\alpha = \sum_\beta L_{\alpha,\beta} X_\beta$$

where $L_{\alpha,\beta}$ is a matrix of *transport coefficients* that can depend on $\mathbf{m}, \rho_i, s$. If $L_{\alpha,\beta}$ is symmetric positive-definite, then so is the entropy generation rate.

Parameterization (I)

Split $\boldsymbol{\sigma}^{\mathrm{fr}}$ and Def $\mathbf{u}$ into trace-free and scalar parts as

$$\boldsymbol{\sigma}^{\mathrm{fr}} = \boldsymbol{\sigma}^{\mathrm{fr}(0)} + \frac{1}{3}(Tr\,\boldsymbol{\sigma}^{\mathrm{fr}})\delta \qquad \mathrm{Def}\ \mathbf{u} = (\mathrm{Def}\ \mathbf{u})^{(0)} + \frac{1}{3}(\nabla\cdot\mathbf{u})\delta$$

with unit diagonal tensor δ and trace-free $\boldsymbol{\sigma}^{\mathrm{fr}(0)}$ and $(\mathrm{Def}\ \mathbf{u})^{(0)}$.
Applying *Curie's principle* gives separate sets of transport coefficients for each type (scalar, vector, tensor) of process

Scalar processes (bulk viscosity, phase changes, cross-phenomena)

$$\begin{bmatrix} Tr\,\boldsymbol{\sigma}^{\mathrm{fr}} \\ -j_i \end{bmatrix} = \begin{bmatrix} \mathcal{L}_{00} & \mathcal{L}_{0j} \\ \mathcal{L}_{i0} & \mathcal{L}_{ij} \end{bmatrix} \begin{bmatrix} \frac{1}{3}\nabla\cdot\mathbf{u} \\ \mu_j \end{bmatrix}$$

Vector processes (heat conduction, diffusion, Soret and Dufour cross effects)

$$-\begin{bmatrix} \mathbf{j}_{\mathrm{s}} \\ \mathbf{j}_{\mathrm{i}} \end{bmatrix} = \begin{bmatrix} L_{ss} & L_{sj} \\ L_{is} & L_{ij} \end{bmatrix} \begin{bmatrix} \nabla T \\ \nabla\mu_j \end{bmatrix}$$

Tensor process (shear viscosity)

$$\boldsymbol{\sigma}^{\mathrm{fr}(0)} = 2\mu(\mathrm{Def}\ \mathbf{u})^{(0)}$$

Parameterization (II)

$$\boldsymbol{\sigma}^{\mathrm{fr}} = 2\mu \mathrm{Def}\ \mathbf{u} + (\frac{1}{9}\mathcal{L}_{00} - \frac{2}{3}\mu)\nabla \cdot \mathbf{u}\,\delta + \frac{1}{3}\sum_i \mathcal{L}_{0i}\,\mu_i \delta$$

with shear viscosity coefficient $\mu \geqslant 0$ and bulk viscosity coefficient $\zeta = \frac{1}{9}\mathcal{L}_{00}$. The *Onsager-Casimir reciprocal relationships* give

$$L_{si} = L_{is} \qquad L_{ij} = L_{ji}$$
$$\mathcal{L}_{0i} = -\mathcal{L}_{i0} \qquad \mathcal{L}_{ij} = \mathcal{L}_{ji}$$

The *mass control conditions* $\sum_i \mathbf{j}_\mathrm{i} = 0$ and $\sum_i j_i = 0$ give

$$\sum_i L_{is} = \sum_i L_{ij} = 0 \qquad \forall j$$
$$\sum_i \mathcal{L}_{i0} = \sum_i \mathcal{L}_{ij} = 0 \qquad \forall j$$

Taken together, the mass control conditions and Onsager-Casimir relationships ensure that $L_{\alpha,\beta}$ and $\mathcal{L}_{\alpha,\beta}$ are positive-definite
$\rightarrow I \geqslant 0 \rightarrow (\mathrm{S}, \mathrm{S}) \geqslant 0 \longrightarrow$ 2nd law of thermodynamics

Connections to Gassmann et. al (2015)

Making the formal identifications (in the case without precipitation)

$$\begin{array}{ccccc} T & \to & \hat{T} & l \to \sigma & \boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u} \to \varepsilon_{sh} \\ \mathbf{j_s}^h & \to & \mathbf{J}_s & \mathbf{j_i} \to \mathbf{J}_i^* & \mu_i \to \hat{\mu}_i \\ j_i & \to & l_i & \eta_i \to \hat{s}_i & q_i \to \hat{q}_i \\ \rho & \to & \bar{\rho} & \mathbf{u} \to \hat{\mathbf{v}} & \boldsymbol{\sigma}^{\mathrm{fr}} \to -\overline{\rho v'' v''} \end{array}$$

in $\partial_t s$ and TI it is easy to show that the two key equations (20) and (28) from Gassmann et. al (2015) are recovered

1. However, interpretation is very different: Gassmann et. al (2015) works with turbulence-averaged quantities, and irreversible processes are interpreted as turbulence closures
2. Also differences in how thermodynamic forces are parameterized, but entropy generation rate is still positive
3. Have not yet worked out how Gassmann (2018) fits into this framework, but we believe it can be done

Overcoming Limitations and Future Work

More Complete Description of Physical System

1. Multiple $\mathbf{u}$ and T (precipitation)
2. Open boundaries (precipitation, lower boundary)
3. Chemical reactions, radiation
4. Turbulence averaging: conditional filtering/multi-fluid? Lagrangian averaging? convected fluid microstructure? EDMF?

Future Work and Extensions

1. Numerical discretization: Quasi-Metriplectic
2. Metriplectic analogue of Energy-Casimir theory
3. Semi-compressible fluids: Anelastic, Pseudo-Incompressible, Boussinesq, Semi-Hydrostatic
4. Non-Eulerian Vertical Coordinates + Quasi-Hydrostatic Approximation

Summary and Conclusions

1. New variational principle gives consistent (1st and 2nd law of thermodynamics) Lagrangian description of geophysical fluids with irreversible processes: requires only a Lagrangian $\mathcal{L}$ and entropy generation rates
2. Corresponding bracket-type formulation is a metriplectic formulation:

$$\frac{\mathsf{d}\mathsf{F}}{\mathsf{d}t} = \{\mathsf{F},\mathsf{H}\} + (\mathsf{F},\mathsf{S})$$

$$\{\mathsf{H},\mathsf{H}\} = 0 \qquad \{\mathsf{S},\mathsf{H}\} = 0$$

$$(\mathsf{H},\mathsf{S}) = 0 \qquad (\mathsf{S},\mathsf{S}) \geqslant 0$$

3. Parameterization can be done such that $(\mathsf{S},\mathsf{S}) \geqslant 0$, requires positive-definite transport coefficient $L_{\alpha,\beta}$

Physics-Dynamics ~~Coupling~~ Decoupling

(Very Incomplete) List of References

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Thanks for Listening! Questions?

Additional Slides

Curl-Form: Lagrangian Reversible

Instead of $\mathbf{m}$, we can predict $\mathbf{v} = \frac{1}{\rho}\frac{\delta \mathcal{L}}{\delta \mathbf{u}}$ instead, which gives the Euler-Lagrange equations

$$\partial_t \left(\frac{1}{\rho}\frac{\delta \mathcal{L}}{\delta \mathbf{u}}\right) + \mathsf{L}_{\mathbf{u}} \left(\frac{1}{\rho}\frac{\delta \mathcal{L}}{\delta \mathbf{u}}\right) - \sum_i q_i \nabla \frac{\delta \mathcal{L}}{\delta \rho_i} - \eta \nabla \frac{\delta \mathcal{L}}{\delta s} = 0,$$

where the Lie derivative is $\mathsf{L}_{\mathbf{u}}\mathbf{v} = \nabla \times \mathbf{v} \times \mathbf{u} + \nabla(\mathbf{u} \cdot \mathbf{v})$, supplemented with the kinematic equations

$$\partial_t \rho_i + \nabla \cdot (q_i \rho\, \mathbf{u}) = 0 \qquad \partial_t s + \nabla \cdot (\eta \rho\, \mathbf{u}) = 0$$

Introducing

$$T := -\frac{\delta \mathcal{L}}{\delta s} \qquad B_i := \mathbf{u} \cdot \mathbf{v} - \frac{\delta \mathcal{L}}{\delta \rho_i} \qquad \mathbf{F} := \rho\, \mathbf{u}$$

gives

$$\partial_t \mathbf{v} + \mathbf{Q} \times \mathbf{F} + \sum_i q_i \nabla B_i + \eta \nabla T = 0$$

$$\partial_t \rho_i + \nabla \cdot (q_i \mathbf{F}) = 0 \qquad \partial_t s + \nabla \cdot (\eta\, \mathbf{F}) = 0$$

These are connected to the curl-form Hamiltonian formulation

Curl-Form: Hamiltonian Reversible

A change of variables from $(\mathbf{m}, \rho_i, s)$ to $(\mathbf{v}, \rho_i, s)$ gives the chain rule for $\mathcal{A}[\mathbf{v}, \rho_i, s] = \mathsf{A}[\mathbf{m}, \rho_i, s]$

$$\frac{\delta \mathcal{A}}{\delta \rho_i} = \frac{\delta \mathsf{A}}{\delta \rho_i} + \mathbf{v} \cdot \frac{\delta \mathsf{A}}{\delta \mathbf{m}} \qquad \frac{\delta \mathcal{A}}{\delta \mathrm{v}} = \rho \frac{\delta \mathsf{A}}{\delta \mathbf{m}} \qquad \frac{\delta \mathcal{A}}{\delta s} = \frac{\delta \mathsf{A}}{\delta s}$$

which yields the functional derivatives

$$\frac{\delta \mathcal{H}}{\delta \mathbf{v}} := \mathbf{F} = \rho\, \mathbf{u} \qquad \frac{\delta \mathcal{H}}{\delta \rho_i} := B_i = \mathbf{u} \cdot \mathbf{v} - \frac{\delta \mathcal{L}}{\delta \rho_i} \qquad \frac{\delta \mathcal{H}}{\delta s} := -\frac{\delta \mathcal{L}}{\delta s}$$

The curl-form Poisson bracket is

$$\{\mathcal{A}, \mathcal{B}\} = -\int_\Omega \frac{\delta \mathcal{A}}{\delta \mathbf{v}} \cdot \left(\mathbf{Q} \times \frac{\delta \mathcal{B}}{\delta \mathbf{v}} \right) \mathrm{d}x$$
$$- \int_\Omega q_i \left(\frac{\delta \mathcal{A}}{\delta \mathbf{v}} \cdot \nabla \frac{\delta \mathcal{B}}{\delta \rho_i} - \frac{\delta \mathcal{B}}{\delta \mathbf{v}} \cdot \nabla \frac{\delta \mathcal{A}}{\delta \rho_i} \right) \mathrm{d}x$$
$$- \int_\Omega \eta \left(\frac{\delta \mathcal{A}}{\delta \mathbf{v}} \cdot \nabla \frac{\delta \mathcal{B}}{\delta s} - \frac{\delta \mathcal{B}}{\delta \mathbf{v}} \cdot \nabla \frac{\delta \mathcal{A}}{\delta s} \right) \mathrm{d}x$$

where $\mathbf{Q} = \frac{\nabla \times \mathbf{v}}{\rho}$.

Curl-Form: Specific Reversible

For multicomponent, multiphase fluids the specific Hamiltonian yields

$$\frac{\delta\mathcal{H}}{\delta\mathbf{v}} := \mathbf{F} = \rho\,\mathbf{u} \qquad \frac{\delta\mathcal{H}}{\delta\rho_i} := B_i = K + \Phi + \mu_i \qquad \frac{\delta\mathcal{H}}{\delta s} := T$$

which give the equations of motion in common form as

$$\begin{gathered}
\partial_t\,\mathbf{u} + \nabla\times\mathbf{u}\times\mathbf{u} + 2\boldsymbol{\Omega}\times\mathbf{u} + \nabla K + \nabla\Phi + \alpha\nabla p = 0 \\
\partial_t\rho_i + \nabla\cdot(q_i\rho\,\mathbf{u}) = 0 \\
\partial_t s + \nabla\cdot(\eta\rho\,\mathbf{u}) = 0
\end{gathered}$$

where we have used $\nabla\times\mathbf{v}\times\mathbf{u} = \nabla\times\mathbf{u}\times\mathbf{u} + 2\boldsymbol{\Omega}\times\mathbf{u}$, $\partial_t\,\mathbf{v} = \partial_t\,\mathbf{u}$ and

$$\sum_i q_i\nabla B_i + \eta\nabla T = \nabla K + \nabla\Phi + \alpha\nabla p$$

since $\sum_i q_i = 1$ and $\sum_i q_i\nabla\mu_i + \eta\nabla T = \alpha\nabla p$ by Gibbs-Duhem

The curl-form metric bracket is

$$(\mathcal{A},\mathcal{B}) = \int \frac{1}{\rho}\frac{\delta\mathcal{A}}{\delta s}\operatorname{div}\boldsymbol{\sigma}^{\mathrm{fr}}\cdot\frac{\delta\mathcal{B}}{\delta\mathbf{v}} + \int \frac{1}{\rho}\frac{\delta\mathcal{B}}{\delta s}\operatorname{div}\boldsymbol{\sigma}^{\mathrm{fr}}\cdot\frac{\delta\mathcal{A}}{\delta\mathbf{v}}$$
$$+ \int \frac{1}{T}\frac{\delta\mathcal{A}}{\delta s}\frac{\delta\mathcal{B}}{\delta s}\left(\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla\mathbf{u} - \operatorname{div}(T\,\mathbf{j}_{\mathrm{s}})\right)$$
$$+ \sum_i \int \frac{\delta\mathcal{A}}{\delta s}(-\operatorname{div}\mathbf{j}_{\mathrm{i}} + j_i)\frac{\delta\mathcal{B}}{\delta\rho_i} + \sum_i \int \frac{\delta\mathcal{B}}{\delta s}(-\operatorname{div}\mathbf{j}_{\mathrm{i}} + j_i)\frac{\delta\mathcal{A}}{\delta\rho_i}$$
$$+ \sum_i \int \frac{1}{T}\frac{\delta\mathcal{A}}{\delta s}\left(-\mathbf{j}_{\mathrm{i}}\cdot\nabla\mu_i - j_i\mu_i\right)\frac{\delta\mathcal{B}}{\delta s}$$

This gives the equations of motion as

$$\partial_t\,\mathbf{v} + \cdots - \frac{1}{\rho}\nabla\cdot\boldsymbol{\sigma}^{\mathrm{fr}} = 0$$
$$\partial_t\rho_i + \cdots + \nabla\cdot\mathbf{j}_{\mathrm{i}} - j_i = 0$$
$$\partial_t s + \cdots + \nabla\cdot\mathbf{j}_{\mathrm{s}} - \frac{1}{T}\boldsymbol{\sigma}^{\mathrm{fr}} : \nabla\mathbf{u} + \frac{1}{T}\mathbf{j}_{\mathrm{s}}\cdot\nabla T + \frac{1}{T}\sum_i(\mathbf{j}_{\mathrm{i}}\cdot\nabla\mu_i + j_i\mu_i) = 0$$

Single Generator Metric Bracket + Beris & Edwards

Evolution of $\mathsf{F}[\mathbf{m}, \rho_i, s]$ is governed by

$$\frac{\mathrm{dF}}{\mathrm{d}t} = \{\mathrm{F}, \mathrm{H}\} + [\mathrm{F}, \mathrm{H}]$$

where the *metric bracket* $[\mathrm{F}, \mathrm{H}]$ is linear in F, possibly nonlinear in H and satisfies $[\mathrm{H}, \mathrm{H}] = 0$ and $[\mathrm{S}, \mathrm{H}] \geqslant 0$

$$[\mathrm{F}, \mathrm{H}] = -\int \nabla \frac{\delta \mathrm{F}}{\delta \mathbf{m}} : \boldsymbol{\sigma}^{\mathrm{fr}}(\frac{\delta \mathrm{H}}{\delta x}) + \sum_i \frac{\delta \mathrm{F}}{\delta \rho_i}(-\nabla \cdot \mathbf{j}_{\mathrm{i}}(\frac{\delta \mathrm{H}}{\delta x}) + j_i(\frac{\delta \mathrm{H}}{\delta x}))$$
$$+ \frac{1}{\frac{\delta \mathrm{H}}{\delta s}} \frac{\delta \mathrm{F}}{\delta s}\Big[- \nabla \cdot (\mathbf{j}_{\mathrm{s}}(\frac{\delta \mathrm{H}}{\delta x})\frac{\delta \mathrm{H}}{\delta s}) + \boldsymbol{\sigma}^{\mathrm{fr}}(\frac{\delta \mathrm{H}}{\delta x}) : \nabla \frac{\delta \mathrm{H}}{\delta \mathbf{m}}$$
$$+ \sum_i \mathbf{j}_{\mathrm{i}}(\frac{\delta \mathrm{H}}{\delta x}) \cdot \nabla \frac{\delta \mathrm{H}}{\delta \rho_i} + \mathbf{j}_{\mathrm{i}}(\frac{\delta \mathrm{H}}{\delta x})\frac{\delta \mathrm{H}}{\delta \rho_i}\Big]$$

with $x = (\mathbf{m}, \rho_i, s)$. For a single component, this reduces to the Beris & Edwards (1998) single generator formalism.

Double Generator and Metriplectic Metric Brackets

1. **Kaufman (1984) Axioms**: linearity, symmetry and $(S, S) \geqslant 0$, $(H, S) = 0$
2. **Metriplectic/GENERIC**: linearity, symmetry and $(S, S) \geqslant 0$, $(H, A) = 0$. The single component version is Morrison (1984).
3. Only difference is $(H, A) = 0$ vs. $(H, S) = 0$
4. **On physical grounds, macroscopic systems require even weaker set**: linearity, $(H, S) = 0$ and $(S, S) \geqslant 0$. However, **microscopic systems** seems to require the full metriplectic axioms, which are connected to the fluctuation-dissipation theorem and transport coefficients.

In all known examples for compressible fluids, metriplectic brackets (GENERIC) require specifying the parameterization of thermodynamic fluxes in terms of forces, while the single generator formalism and Kaufman's axioms do not.

Start by rewriting $\nabla \mu_i$ and $\mathbf{j}_\mathsf{s}$ as

$$\nabla \mu_i = \nabla \mu_i|_T - \eta_i \nabla T \qquad \mathbf{j}_\mathsf{s} = \frac{{\mathbf{j}_\mathsf{s}}^h}{T} + \sum_i \eta_i \, \mathbf{j}_\mathsf{i}$$

with $\nabla \mu_i|_T$ the gradient of $\mu_i(p, q_i, T)$ with T held constant, $\eta_i = \frac{\partial \eta}{\partial q_i}(p, T, q_i)$ the partial specific entropy and ${\mathbf{j}_\mathsf{s}}^h$ the sensible heat flux. Using these, we can rewrite $\partial_t s$ and the entropy generation rate TI as

$$\partial_t s + \cdots + \nabla \cdot (\frac{{\mathbf{j}_\mathsf{s}}^h}{T} + \sum_i \eta_i \, \mathbf{j}_\mathsf{i}) - \frac{1}{T} \boldsymbol{\sigma}^{\mathrm{fr}} : \nabla u + \frac{{\mathbf{j}_\mathsf{s}}^h}{T^2} \cdot \nabla T$$

$$+ \frac{1}{T} \sum_i \mathbf{j}_\mathsf{i} \cdot \nabla \mu_i|_T + j_i \mu_i = 0$$

$$TI = \boldsymbol{\sigma}^{\mathrm{fr}} : \nabla \mathbf{u} - \frac{{\mathbf{j}_\mathsf{s}}^h}{T} \cdot \nabla T - \sum_i \mathbf{j}_\mathsf{i} \cdot \nabla \mu_i|_T + j_i \mu_i$$

Parameterization: Atmosphere Specific (II)

Express vectorial processes using
–fluxes: sensible heat flux $\mathbf{j}_\mathrm{s}{}^h = T(js - \sum_i \eta_i \mathbf{j}_\mathrm{i})$, diffusion flux $\mathbf{j}_\mathrm{i}$ (instead of $\mathbf{j}_\mathrm{s}$,$\mathbf{j}_\mathrm{i}$)
–forces: $\frac{\nabla T}{T}$, $\nabla \mu_i | T$ (instead of ∇T,$\nabla \mu_i$)
Gives a parameterization

$$\begin{bmatrix} \mathbf{j}_\mathrm{s}{}^h \\ \mathbf{j}_\mathrm{i} \end{bmatrix} = \begin{bmatrix} A_{ss} & A_{sj} \\ A_{is} & A_{ij} \end{bmatrix} \begin{bmatrix} \frac{\nabla T}{T} \\ \nabla \mu_i |_T \end{bmatrix}.$$

where

$$\mathrm{A} = \mathrm{MLM}^T, \quad \text{for} \quad \mathrm{M} = \begin{bmatrix} T & -T\eta_1 & -T\eta_2 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}.$$

Since M is invertible ($T > 0$), L is SPD iff M is SPD $\rightarrow$ apply same rules (Onsager-Casimir reciprocal relations, mass control conditions) to A_{ij} as L_{ij}

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