Entropy, Dissipation and Lagrangian Hydrodynamics

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PLAN OF THE TALK 1/2

• **Background**: from differential equations to algebræ of observables for Hamiltonian (conservative) systems via symplectic brackets. **Problem**: friction breaks the symplectic framework;

• **Algebrizing friction via the metriplectic formalism**: complete systems, Hamiltonian, entropy and metriplectic algebræ;

• **Lagrangian formalism in fluids and parcel variables**: from the 6N particle variables to the 6 parcel centre-of-mass variables, plus entropy of the relative variables;

• **Ideal fluids**: equations of motion, Lagrangian and Hamiltonian formulations;

• **Mechanism of dissipation**: friction between two nearby parcels and heat conduction. Equations of motion of non-ideal fluids;
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• **Non-ideal fluids:** the metriplectic formulation;

• Conclusions.
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- **Background**: from differential equations to algebræ of observables for Hamiltonian (conservative) systems via symplectic brackets.

**Problem**: friction breaks the symplectic framework;
**Algebrizing dynamical systems:** defining a suitable product, turning the set of observables into a closed algebra $O$ that prescribes the whole dynamics.

**Extended definition of (non-canonical) Hamiltonian dynamics** for a general dynamical system:

$$\dot{\psi} = F(\psi) \quad / \quad \psi \in \mathbb{V}$$

- there exists a **conserved total energy** (candidate Hamiltonian $H$):

  $$\exists \quad H(\psi) \quad / \quad [H] = m\ell^2 t^{-2}, \quad \dot{H} \triangleq 0$$

- there exists a **good Poisson bracket** (antisymmetric 2-form on the manifold of the motions satisfying Jocobi’s identity), so that the motion is generated by it as:

  $$\dot{f} \triangleq \partial_t f + \{f, H\} \quad \forall \quad f = f(\psi)$$
Gifts of algebrization:

Identification of symmetries with conservation laws

Straightforward implementation of continuous groups

Exact constraints for numerical schemes: Casimir quantity method

Orbit diagnosis without solving the equations!

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WHAT ABOUT FRICTION?

Friction has to do with:

- **Stopping** (i.e., asymptotic stability);

- **Warming up** (i.e., heat production/transfer, i.e. irreversibility-entropy);

- **Mechanical energy dissipation** (i.e., breakup of the Hamiltonian framework);

- **Thermodynamics** arising naturally from mechanics (i.e., microscopic degrees of freedom treated statistically)

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Friction breaks down the Hamiltonian framework for various reasons:

- Friction drives systems to asymptotic equilibria, shrinking the phase space volume...

...while Hamiltonian systems conserve phase space volumes;

- Mechanical energy is worn out by friction, so what may play the role of Hamiltonian?
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Dissipation involves the environment, hence rendering the primitive algebra $O$ unable to predict the whole dynamics. $O$ remains incomplete.
Need of **completing the dissipative system**, in order to algebrize it:

- **including “the environment”;**
- **re-defining a suitably generalized product \( \langle\langle f, g\rangle\rangle; \)**
- **defining a new quantity \( F \) generating the dissipative motion**

\[
\langle\langle A_i'', A_j'' \rangle \rangle = \phi_{ij}'' (A_1'', \ldots, A_N'') \quad \forall \quad A_i'', A_j'' \in \mathcal{O}''
\]

Completing the system means closing it including the interacting environment: **need of environmental observables**
Environmental observables must have statistical nature: friction is a heat exchange with the environment, hence statistics of the variables describing the latter arise naturally.

“Environmental quantities” completing the system will describe microscopic statistically treated degrees of freedom (μSTDOF): a complete system will be described as \((\psi_{\text{macro}}, P(\psi_{\text{micro}}))\)
The closed algebra \( (O'', \langle\langle*, *\rangle\rangle) \) includes the space-time transformation generators (energy \( H \), momenta, boost generators) and the entropy of the \( \mu \)STDOF.

Prigogine’s approach: the entropy is a form of Lyapunov function, related to the dissipative component of dynamics.

Metric systems are intrinsically irreversible, very easily algebraized and show asymptotic equilibria and Lyapunov observables:

\[
\dot{\psi}_h = \Gamma_{hk}(\psi) \frac{\partial K(\psi)}{\partial \psi_k} \quad / \quad \det \|\Gamma_{hk}(\psi)\| \geq 0, \quad \Gamma_{hk} = \Gamma_{kh}
\]
*K is a Lyapunov, monotonic in time* along the motion, hence the system is irreversible (and asymptotically in equilibrium wherever *K* is stationary):

\[
\dot{K}(\psi) = \frac{\partial K(\psi)}{\partial \psi_h} \cdot \psi_h = \frac{\partial K(\psi)}{\partial \psi_h} \Gamma_{hk}(\psi) \frac{\partial K(\psi)}{\partial \psi_k} \geq 0 \quad \forall \quad \psi
\]

A symmetric (positive-)semidefinite 2-form \((f,g)\) may be defined producing the motion for the metric dynamics:

\[
(f,g) = \Gamma_{hk} \frac{\partial f}{\partial \psi_h} \frac{\partial g}{\partial \psi_k}, \quad \dot{f} = \partial_t f + (f, K)
\]

**Hamiltonian systems plus friction:** the algebrization of the dissipative component will make use of a metric algebra, with \(K = S\). The Hamiltonian component will still be symplectic.

The metric component will be the one prevailing near a local asymptotic equilibrium (overdamped limit).
How should a metric and a symplectic structure co-exist?

• The total energy generates symplectically the non-dissipative limit of the system, and in that purely Hamiltonian limit the total entropy should remain constant:

\[ \{S, H\} = 0 \]

• The total entropy is the Lyapunov function generating metrically the dissipative part of the system, that does not alter the total energy:

\[(S, H) = 0\]

• The total entropy increases due to the dissipative part of the system:

\[ \alpha(S, S) \geq 0 \]

These requirements are met by the metriplectic formalism (MF), that puts together the Hamiltonian-conservative-symplectic and the entropic-dissipative-metric parts of the motion.
**Metriplectic algebra:** the gradients of observables are composed to give other observables by a bi-linear algebra which is partially symplectic and partially metric

\[ \langle \langle f, g \rangle \rangle = \{ f, g \} + (f, g) \quad \forall \quad f = f(\psi), \quad g = g(\psi) \]

**Metriplectic motion via free energy:** a linear combination \( F \) (free energy) of \( H \) and \( S \) is constructed

\[ F = H + \alpha S \]

and the dynamics is prescribed to be **metriplectically generated by** \( F \):

\[ \dot{f} = \partial_i f + \langle \langle f, F \rangle \rangle \quad \forall \quad f = f(\psi), \]

\[ \dot{\psi}(\psi_0) = 0 \quad \iff \quad \frac{\partial F(\psi_0)}{\partial \psi_i} = 0 \]
\[ \dot{f} = \partial_t f + \langle \langle f, F \rangle \rangle \]

Habemus Algebream...

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$S$ of the $\mu$STDOF changes **only due to the dissipation terms**. In order for $S$ to have naturally zero Poisson bracket with $H$, it is expected to be a function of the Casimir quantities:

$$\{C_\alpha, f\} = 0 \quad \forall \quad f = f(\psi), \quad S = S(C_1, \ldots, C_n) \quad \Rightarrow \quad \{S, H\} = 0$$

**Metric bracket**: a symmetric, semi-definite 2-form on the gradients of the observables, which has $H$ as a “null mode”:

$$\Gamma_{ij} \frac{\partial H}{\partial \psi_i} \frac{\partial f}{\partial \psi_j} = 0 \quad \forall \quad f = f(\psi) \quad \Rightarrow \quad (S, H) = 0$$

Since $S$ is a Casimir and $H$ has zero metric bracket with anything, one has:

$$\dot{f} = \partial_i f + \{f, H\} + \alpha (f, S) \quad \forall \quad f = f(\psi)$$
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• Lagrangian formalism in fluids and parcel variables: from the 6N particle variables to the 6 parcel centre-of-mass variables, plus entropy of the relative variables;
The fluid system is represented as a continuum domain evolving with time. It is subdivided into infinitely many infinitesimal parcels, initially spanned by a continuous 3D index $\vec{a}$. As the continuum evolves, the parcel positions are $\vec{\zeta}(\vec{a}, t)$.

\[ \vec{\zeta}(\vec{a}, 0) = \vec{a}, \]
\[ J(\vec{a}, t) = \frac{\partial \vec{\zeta}(\vec{a}, t)}{\partial \vec{a}}, \]
\[ \mathcal{J}(\vec{a}, t) = \det J(\vec{a}, t) \]
\[ d^3\zeta(\vec{a}, t) = \mathcal{J}(\vec{a}, t) d^3a \]
\[ \rho(\vec{a}, t) = \frac{\rho_0(\vec{a}, t)}{\mathcal{J}(\vec{a}, t)}. \]
• Each parcel is formed by $N(\vec{a})$ particles, the thermodynamics of which will complete the physics of the parcel crucially.

• The position and momentum of the parcel $\vec{\zeta}$ and $\vec{\pi}$ are the centre-of-mass variables of those $N(\vec{a})$ particles.

$$\vec{\zeta}(\vec{a}, t) = \frac{1}{N(\vec{a})} \sum_{I=1}^{N(\vec{a})} \vec{r}_I(t),$$

$$\vec{\pi}(\vec{a}, t) = \frac{1}{d^3a} \sum_{I=1}^{N(\vec{a})} \vec{p}_I(t) = \rho_0(\vec{a}) \partial_t \vec{\zeta}(\vec{a}, t)$$

• The equilibrium thermodynamics of the particles forming the parcel completes the physical description through the use of the mass-specific entropy density attributed to the parcel:

$$s(\vec{a}, t), \quad U\left(\frac{\rho_0}{\mathcal{F}}, s\right),$$

$$p = -\rho_0 \frac{\partial U}{\partial \mathcal{F}}, \quad T = \frac{\partial U}{\partial s}$$
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• Ideal fluids: equations of motion, Lagrangian and Hamiltonian formulations;
• In the absence of friction and thermal conductivity the parcel is expected to satisfy a mechanical action principle, that requires the survey of all forms of parcel energy to be written:

\[ dE_{\text{kin}} = \frac{\rho_0}{2} \dot{\zeta}^2 d^3 a, \quad dV = \rho_0 \phi \left( \hat{\zeta} \right) d^3 a, \quad dE_{\text{therm}} = \rho_0 U \left( \frac{\rho_0}{f}, s \right) d^3 a, \]

\[
A \left[ \zeta, \dot{\zeta}, s \right] = \int_{t_i}^{t_f} dt \int_{D_0} d^3 a \left[ \frac{\rho_0}{2} \dot{\zeta}^2 - \rho_0 \phi \left( \hat{\zeta} \right) - \rho_0 U \left( \frac{\rho_0}{f}, s \right) \right]
\]

• Euler-Lagrange equations for the Lagrangian degrees of freedom of the fluid read:

\[
\ddot{\zeta}_\alpha = - \frac{\partial \phi \left( \hat{\zeta} \right)}{\partial \zeta_\alpha} - \partial_i \left( p A_\alpha^i \left( \partial \hat{\zeta} \right) \right), \quad A_\alpha^i = \frac{\epsilon_{\alpha \kappa \lambda}}{2} \epsilon_{imn} \partial_m \zeta^K \partial_n \zeta^\lambda,
\]

\[
\ddot{s} = \dot{s} = 0
\]
• Out of the **Lagrangian density** one can write the **Hamiltonian density** via Legendre transform:

\[
\mathcal{L} (\zeta, \dot{\zeta}, s) = \frac{\rho_0}{2} \dot{\zeta}^2 - \rho_0 \phi \left( \bar{\zeta} \right) - \rho_0 \mathcal{U} \left( \frac{\rho_0}{\mathcal{F}}, s \right),
\]

\[
\mathcal{H} (\zeta, \pi, s) = \frac{\pi^2}{2 \rho_0} + \rho_0 \phi \left( \bar{\zeta} \right) + \rho_0 \mathcal{U} \left( \frac{\rho_0}{\mathcal{F}}, s \right)
\]

• **Hamiltonian’s equations of motion** for the position and momentum of the parcel are straightforwardly obtained:

\[
\dot{\zeta}^\alpha = \frac{\pi^\alpha}{\rho_0}, \quad \dot{\pi}_\alpha = - \frac{\partial \varphi \left( \bar{\zeta} \right)}{\partial \zeta^\alpha} - A_\alpha^i \partial_i p
\]

• The evolution (conservation) of the **parcel’s entropy** may be found naturally passing to the algebrization of the ideal fluid...
An “apparently canonical” Poisson bracket is defined for the ideal fluid in the Lagrangian formalism:

\[ \{ F, G \} = \int_{D_0} d^3 a \left[ \frac{\delta F}{\delta \zeta^\alpha (\vec{a})} \frac{\delta G}{\delta \pi^\alpha (\vec{a})} - \frac{\delta G}{\delta \zeta^\alpha (\vec{a})} \frac{\delta F}{\delta \pi^\alpha (\vec{a})} \right] \]

The equations of motion are obtained now through this symplectic algebra:

\[ H [\zeta, \pi, s] = \int_{D_0} \mathcal{H} (\zeta, \pi, s) d^3 a, \quad \dot{\zeta}^\alpha = \{ \zeta^\alpha, H \}, \quad \dot{\pi}_\beta = \{ \pi_\beta, H \}, \quad \dot{s} = \{ s, H \} = 0 \]

Ideal fluids’ parcel entropy is conserved: this may emerge as a consequence of the absence of derivatives with respect to \( s \) in the definition of Poisson bracket. This fact also renders the entropy a Casimir invariant:

\[ S [s] = \int_{D_0} \rho_0 (\vec{a}) s (\vec{a}, t) d^3 a, \]

\[ \{ S, G \} = 0 \quad \forall \quad G \]
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• Ideal fluids: equations of motion, Lagrangian and Hamiltonian formulations;

• Mechanism of dissipation: friction between two nearby parcels and heat conduction. Equations of motion of non-ideal fluids;
• Being to collisions from relative motions, friction between two nearby parcels depends on their velocity difference (gradient). Heat conduction instead depends (linearly) on the temperature difference.

• In the Lagrangian formalism these dissipation terms enter the equations via addenda calculated thanks to the diffeomorphic nature of the continuum motion.

\[
\partial_t \zeta (\tilde{a}, t) + J (\tilde{a}, t) \cdot d\tilde{a}
\]
Equations of motion of the non-ideal fluids in Lagrangian Formalism:

\[ \frac{\dot{\zeta}^\alpha}{\rho_0} = \pi^\alpha, \]

\[ \dot{\pi}^\alpha = -\frac{\partial}{\partial a^i} \left( p A^{\alpha i} \left( \partial \zeta^i \right) \right) - \nabla^\alpha \phi + J \left( \partial \zeta^i \right) \nabla^\eta \sigma^\alpha \eta, \]

\[ \dot{s} = \frac{J \Lambda_{\alpha \beta \gamma \delta}}{\rho_0 T} \nabla^\alpha \left( \frac{\pi^\beta}{\rho_0} \right) \nabla^\gamma \left( \frac{\pi^\delta}{\rho_0} \right) + \frac{\kappa J}{\rho_0 T} \nabla^\eta \nabla^\eta T, \]

\[ \nabla^\alpha \overset{\text{def}}{=} (J^{-1})^\alpha_i \frac{\partial}{\partial a^i}, \quad \sigma_{\alpha \beta} = \Lambda_{\alpha \beta \gamma \delta} (J^{-1})^{k \gamma} \frac{\partial \pi^\delta}{\partial a^k}, \]

\[ \Lambda_{\alpha \beta \gamma \delta} \overset{\text{def}}{=} \eta \left( \delta_{\delta \alpha} \delta_{\gamma \beta} + \delta_{\delta \beta} \delta_{\gamma \alpha} - \frac{2}{3} \delta_{\alpha \beta} \delta_{\gamma \delta} \right) + \zeta \delta_{\alpha \beta} \delta_{\gamma \delta} \]
PLAN OF THE TALK 2/2

- Non-ideal fluids: the metriplectic formulation;
The central result of this presentation, namely the metric bracket for non-ideal fluids in Lagrangian Formalism, is obtained out of the expression of the same quantity in Eulerian formalism:

$$(F, G) =$$

$$= \frac{1}{\lambda} \int_D d^3x \left\{ T \Lambda_{ikmn} \left[ \partial^i \left( \frac{1}{\rho} \frac{\delta F}{\delta v_k} \right) - \frac{1}{\rho T} \partial^i v^k \frac{\delta F}{\delta s} \right] \left[ \partial^m \left( \frac{1}{\rho} \frac{\delta G}{\delta v_n} \right) - \frac{1}{\rho T} \partial^m v^n \frac{\delta G}{\delta s} \right] + \kappa T^2 \partial^k \left( \frac{1}{\rho T} \frac{\delta F}{\delta s} \right) \partial_k \left( \frac{1}{\rho T} \frac{\delta G}{\delta s} \right) \right\}$$

($$\rho, s$$ and $$v$$ are the Eulerian variables mass density, mass-specific entropy density and bulk velocity).
This **caveat** renders it possible to write the **metric bracket in Lagrangian Formalism** as follows:

\[
(F, G) = \\
= \frac{1}{\lambda} \int_{D_0} \mathcal{J} d^3 a \left\{ T \Lambda_{\alpha \beta \gamma \delta} \left[ \nabla^\alpha \left( \frac{\delta F}{\delta \pi_\beta} \right) - \frac{1}{\rho_0 T} \nabla^\alpha \left( \frac{\pi_\beta}{\rho_0} \right) \frac{\delta F}{\delta s} \right] \left[ \nabla^\gamma \left( \frac{\delta G}{\delta \pi_\delta} \right) - \frac{1}{\rho_0 T} \nabla^\gamma \left( \frac{\pi_\delta}{\rho_0} \right) \frac{\delta G}{\delta s} \right] + \right. \\
\left. + \kappa T^2 \nabla^\eta \left( \frac{1}{\rho_0 T} \frac{\delta F}{\delta s} \right) \nabla^\eta \left( \frac{1}{\rho_0 T} \frac{\delta G}{\delta s} \right) \right\}
\]
Entropy generates the dissipative part of momentum and entropy-density dynamics through this metric bracket:

\[
(\hat{\pi}_t (\tilde{a}'))_{\text{diss}} = \lambda (\pi_t (\tilde{a}'), S), \quad (\dot{s} (\tilde{a}'))_{\text{diss}} = \lambda (s (\tilde{a}'), S)
\]

\[
F = H + \lambda S,
\]

\[
H = \int_{D_0} \left[ \frac{\pi^2}{2 \rho_0} + \rho_0 \phi \left( \zeta \right) + \rho_0 U \left( \frac{\rho_0}{\mathcal{J}}, s \right) \right] d^3 a,
\]

\[
S [s] = \int_{D_0} \rho_0 (\tilde{a}) s (\tilde{a}, t) d^3 a,
\]

\[
\dot{\Phi} = \langle\langle \Phi, F \rangle\rangle,
\]

\[
\langle\langle A, B \rangle\rangle = \{A, B\} + (A, B)
\]

\[
\{S, H\} = 0, \quad (S, H) = 0
\]

- A suitable combination of Hamiltonian and entropy, namely the free energy \( F \), gives rise to the full dynamics of the complete system, provided the metriplectic bracket \( \langle\langle...,\rangle\rangle \) is defined.
PLAN OF THE TALK 2/2

• Non-ideal fluids: the metriplectic formulation;

• Conclusions.
• **All the gifts** of the algebrized Physics for the conservative systems.

• **Friction forces**, acting within isolated (complete) systems, are algebrized.

• **Dissipative motion** is produced by a suitable semi-definite symmetric bracket with the entropy of the µSTDOF onto which dissipation pours energy.

• The symmetric bracket plus the Poisson bracket of the conservative motion defines the metriplectic algebra $<[A,B]>$ of the observables of complete systems.

• The metriplectic formalism algebraically generates motions converging to asymptotic equilibria for dissipative isolated systems.
• Fluids in Lagrangian Formalism: the motion of the continuous system is given by the diffeomorphism mapping the initial material domain into the one at a later generic time \( t \);

• Introducing the parcel variables: \( \zeta \) and \( \pi \) describe the dynamics of the centre-of-mass of the parcel, while the relative variables are statistically described by the equilibrium thermodynamics of the parcel’s particles. Dilation factor \( J \) and entropy density;

• Ideal fluids: \( \zeta \) and \( \pi \) are involved in a symplectic dynamics, while the entropy does not change at all, being a Casimir invariant;

• Non-ideal fluids: the formerly define symplectic dynamics is enriched by a metric part, confering to \( \pi \) a dissipative dynamics, while the entropy, remaining a Casimir invariant, monotonically grows due to the metric.
Thank you very much for your kind attention...

...but it’s already time to go.

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