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**;

PLAN OF THE TALK 2/2

- **Non-ideal fluids: the metriplectic formulation;**
- **Conclusions.**

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 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:

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

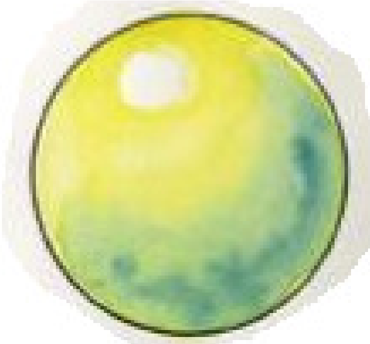
- **there exists a conserved total energy (candidate Hamiltonian *H*):**

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

- **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:**

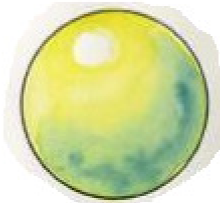
$$\boxed{\dot{f} \overset{\circ}{=} \partial_t f + \{f, H\} \quad \forall \quad f = f(\psi)}$$

Gifts of algebrization:

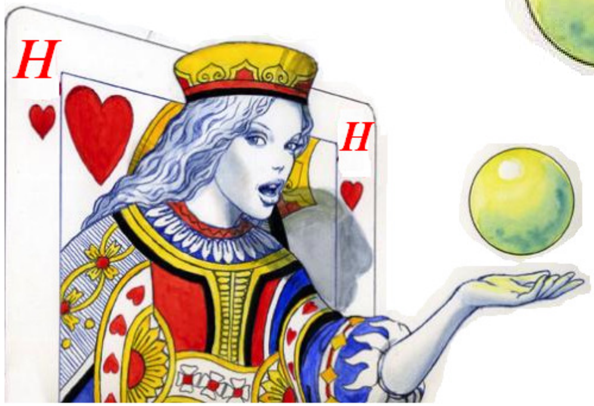


Identification of symmetries with conservation laws

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?

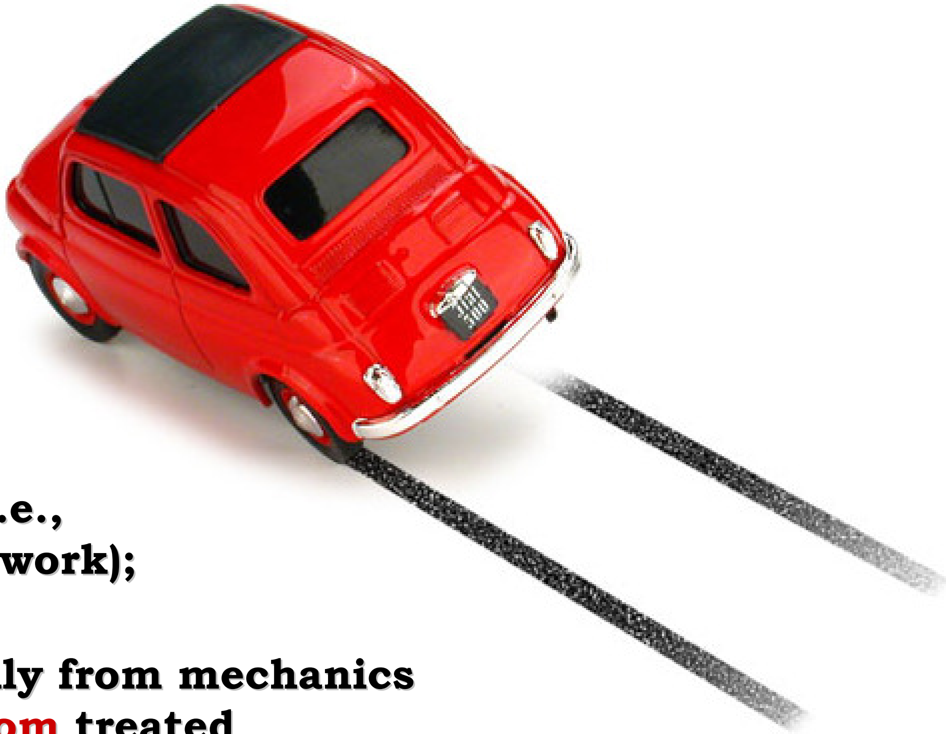
Friction has to do with:

- **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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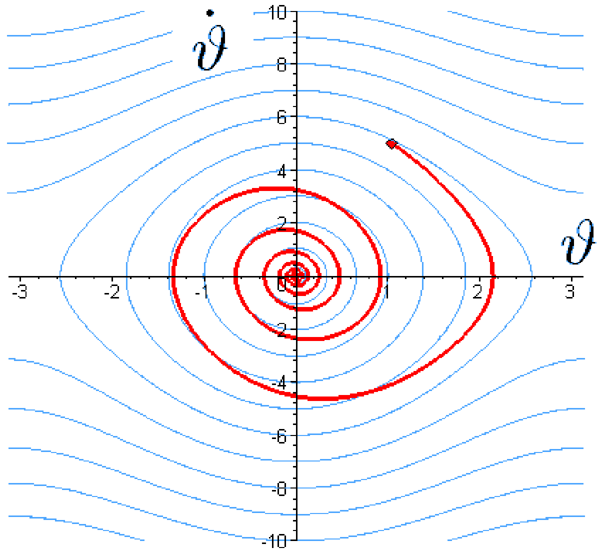
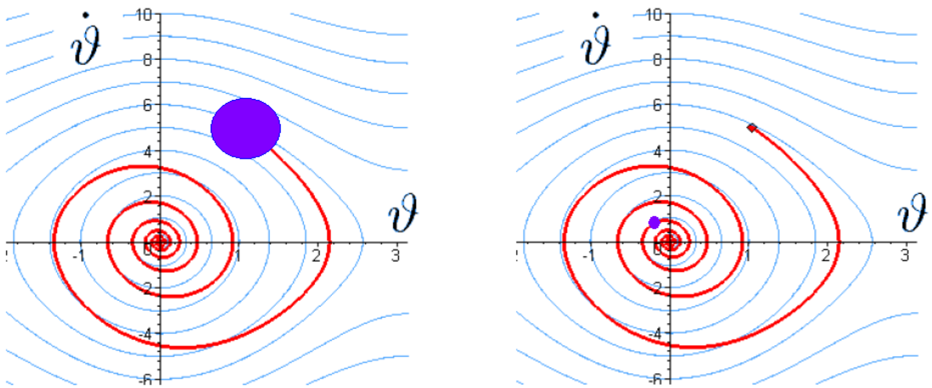
Friction breakes down the Hamiltonian framework for various reasons:



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



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…while Hamiltonian systems conserve phase space volumes;

$$\dot{E} \neq 0$$

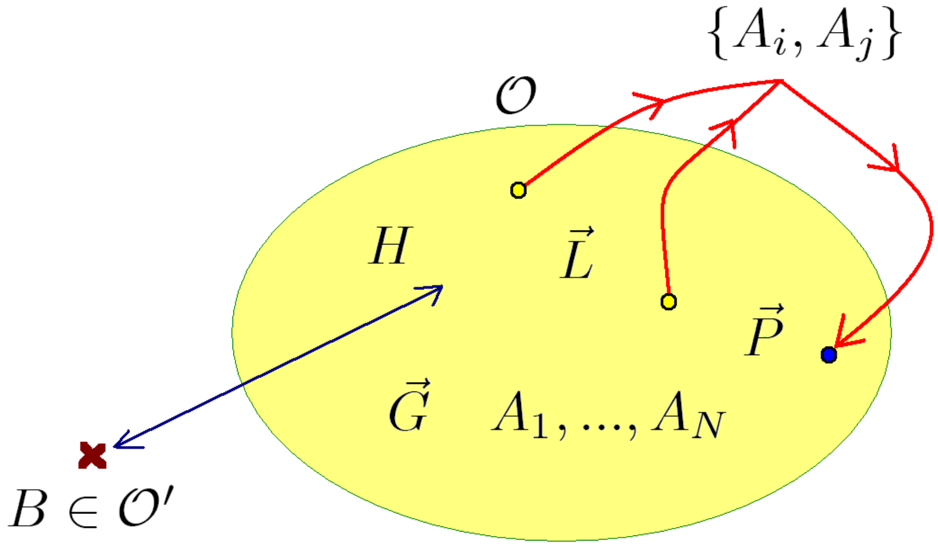
- **Mechanical energy is worn out by friction, so what may play the role of Hamiltonian?**

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;

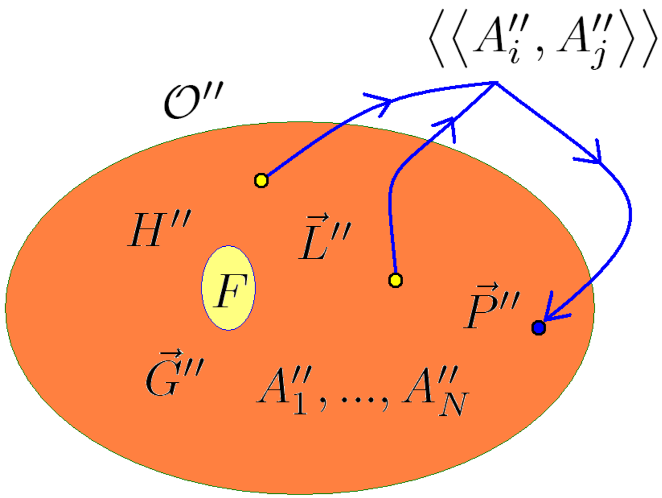
• Algebrizing friction via the metriplectic formalism: complete systems, Hamiltonian, entropy and metriplectic algebræ;

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 <<*f,g*>>;**
- **defining a new quantity *F* generating the dissipative motion**

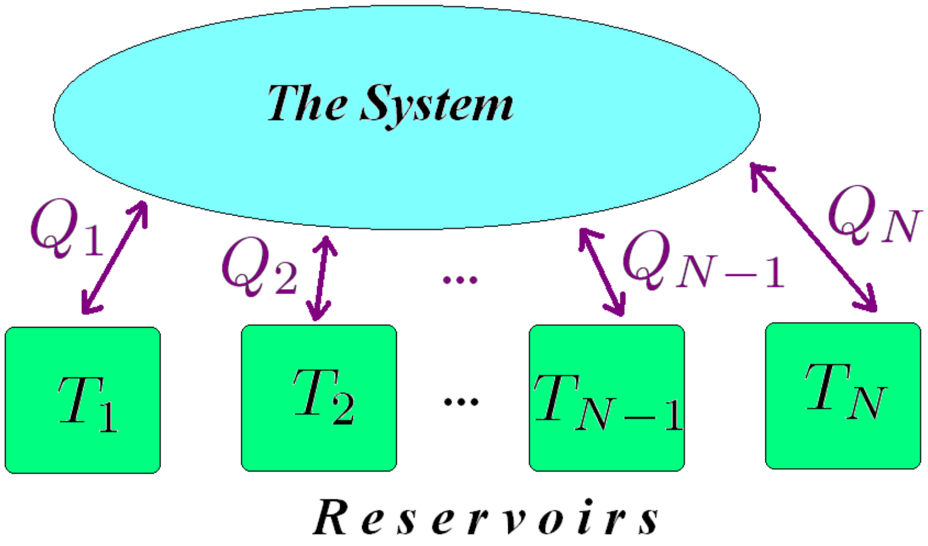


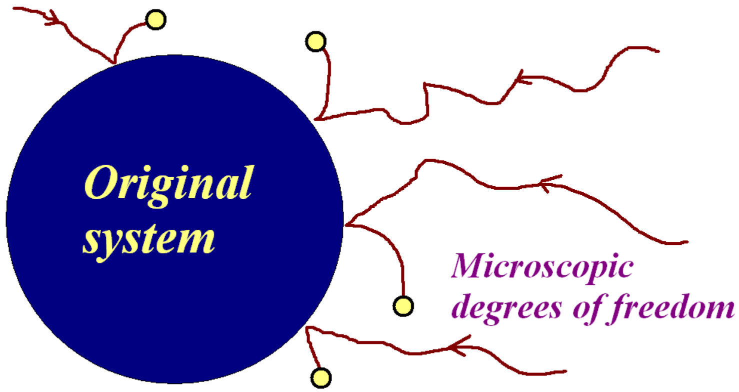
$$\forall \quad A''_i, A''_j \in \mathcal{O}'' \quad \langle\langle A''_i, A''_j \rangle\rangle = \phi''_{ij}\left(A''_1, \ldots, A''_N\right)$$

$$/ \quad \phi''_{ij}\left(A''_1, \ldots, A''_N\right) \in \mathcal{O}''$$

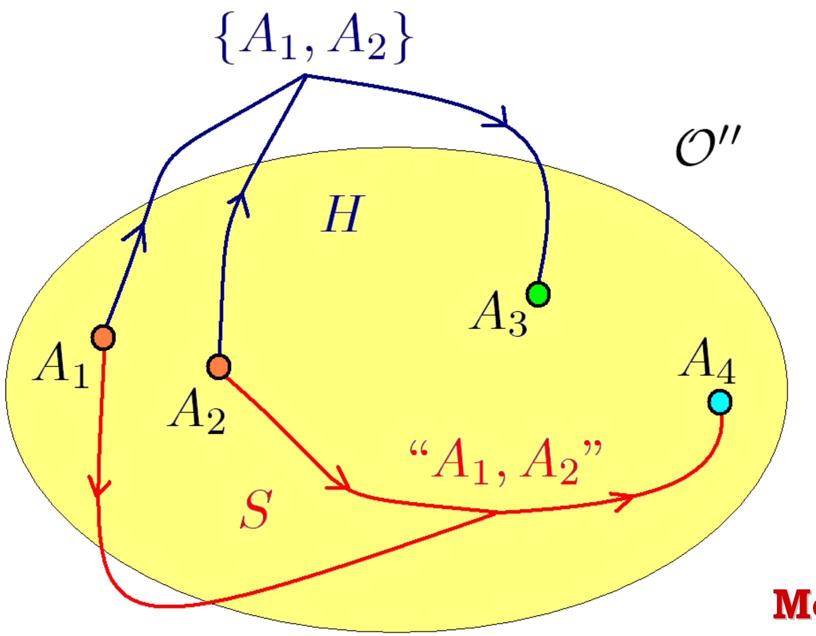
Completing the system means closing it including the interacting environment: need of environmental observables

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 $(\psi_{macro}, P(\psi_{micro}))$



The closed algebra (*O''*,<<*,*>>) inlcudes the space-time transformation generators (energy *H*, momenta, boost generators) and the entropy of the μSTDOF.

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 algebrized 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):

$$\dot{K}(\psi) = \frac{\partial K(\psi)}{\partial \psi_h} \dot{\psi}_h = \frac{\partial K(\psi)}{\partial \psi_h} \Gamma_{hk}(\psi) \frac{\partial K(\psi)}{\partial \psi_k} \geq 0 \quad \forall \quad \psi$$

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

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

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***:

$$\dot{f} = \partial_t f + \langle\langle f,F\rangle\rangle \quad \forall \quad f = f(\psi)\,,$$

$$\dot{\psi}(\psi_0) = 0 \quad \Longleftrightarrow \quad \frac{\partial F(\psi_0)}{\partial \psi_i} = 0$$

$$\dot{f} = \partial_t f + \langle\langle f, F \rangle\rangle$$

Habemus Algebram...

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S **of the μSTDOF 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:**

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

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:

$$\dot{f} = \partial_t f + \{f, H\} + \alpha (f, S) \quad \forall \quad f = f(\psi)$$

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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;

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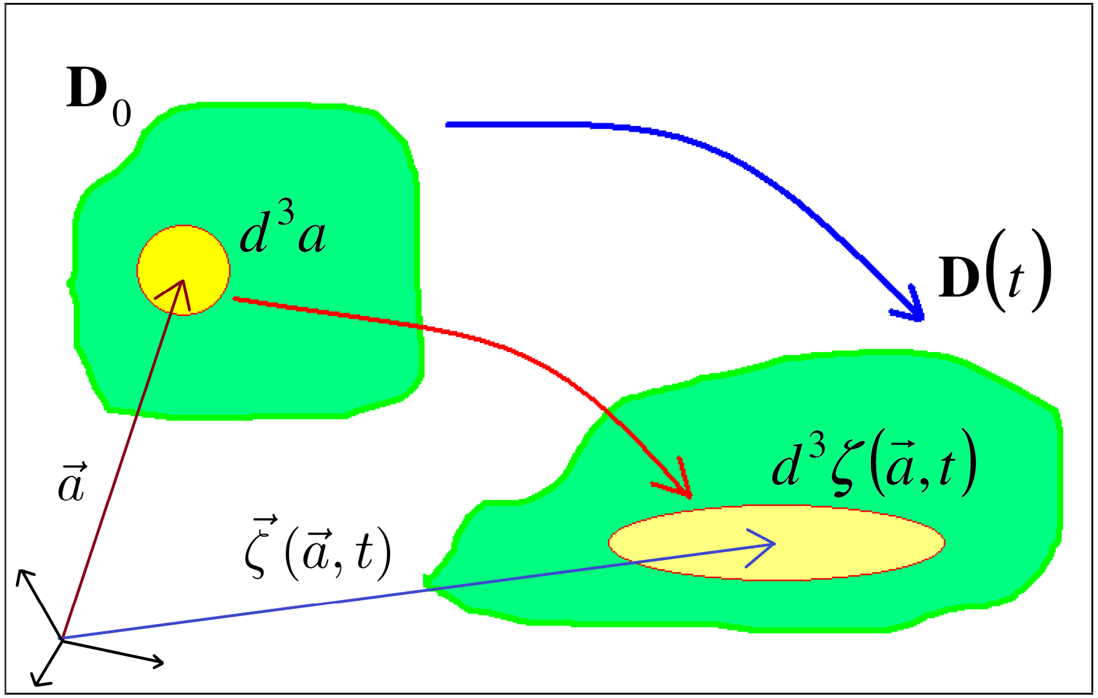
• Lagrangian formalism in fluids and parcel variables: from the 6N particle variables to the 6 parcel centre-of-mass variables, plus entropy of the relative variables;

• **The fluid sytem 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** $\vec{\zeta}\left(\vec{a},t\right)$



$$\vec{\zeta}\left(\vec{a},0\right)=\vec{a},$$

$$J\left(\vec{a},t\right)=\frac{\partial\vec{\zeta}\left(\vec{a},t\right)}{\partial\vec{a}},$$

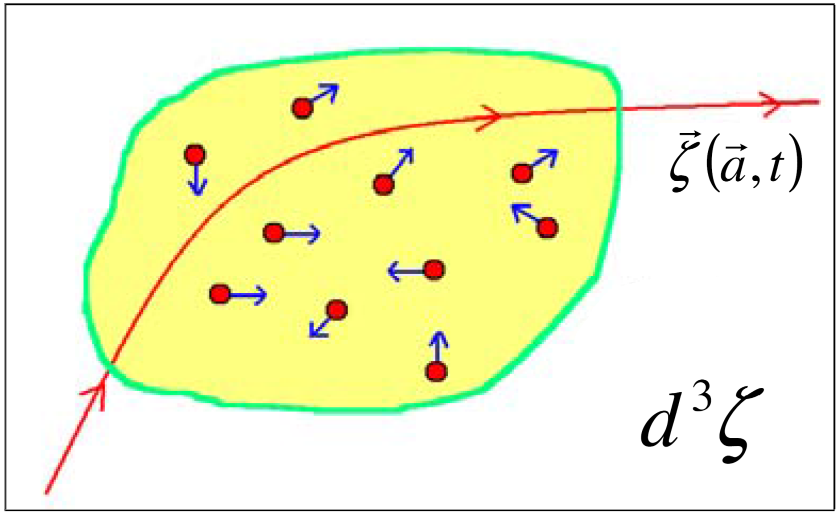
$$\mathcal{J}\left(\vec{a},t\right)=\det J\left(\vec{a},t\right)$$

$$d^3\zeta\left(\vec{a},t\right)=\mathcal{J}\left(\vec{a},t\right)d^3a$$

$$\rho\left(\vec{a},t\right)=\frac{\rho_0\left(\vec{a},t\right)}{\mathcal{J}\left(\vec{a},t\right)}.$$

- **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.**



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

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

- **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:**

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

$$p = -\rho_0 \frac{\partial \mathcal{U}}{\partial \mathcal{J}}, \qquad T = \frac{\partial \mathcal{U}}{\partial s}$$

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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:

$$dE_{\mathrm{kin}} = \frac{\rho_0}{2}\dot{\zeta}^2 d^3a, \quad dV = \rho_0 \phi\left(\vec{\zeta}\right) d^3a, \quad dE_{\mathrm{therm}} = \rho_0 \mathcal{U}\left(\frac{\rho_0}{\mathcal{J}}, s\right) d^3a,$$

$$A\left[\zeta, \dot{\zeta}, s\right] = \int_{t_{\mathrm{i}}}^{t_{\mathrm{f}}} dt \int_{\mathbb{D}_0} d^3a \left[\frac{\rho_0}{2}\dot{\zeta}^2 - \rho_0 \phi\left(\vec{\zeta}\right) - \rho_0 \mathcal{U}\left(\frac{\rho_0}{\mathcal{J}}, s\right)\right]$$

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

$$\ddot{\zeta}_\alpha = -\frac{\partial \phi\left(\vec{\zeta}\right)}{\partial \zeta^\alpha} - \partial_i \left(p A_\alpha{}^i \left(\partial \vec{\zeta}\right)\right), \qquad A_\alpha{}^i = \frac{\epsilon_{\alpha\kappa\lambda}}{2} \epsilon^{imn} \partial_m \zeta^\kappa \partial_n \zeta^\lambda,$$

$$\ddot{s} = \dot{s} = 0$$

• **Out of the Lagrangian density one can write the Hamiltonian density via Legendre transform:**

$$\mathcal{L}\left(\zeta,\dot{\zeta},s\right)=\frac{\rho_0}{2}\dot{\zeta}^2-\rho_0\phi\left(\vec{\zeta}\right)-\rho_0\mathcal{U}\left(\frac{\rho_0}{\mathcal{J}},s\right),$$

$$\mathcal{H}\left(\zeta,\pi,s\right)=\frac{\pi^2}{2\rho_0}+\rho_0\phi\left(\vec{\zeta}\right)+\rho_0\mathcal{U}\left(\frac{\rho_0}{\mathcal{J}},s\right)$$

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

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

• **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:**

$$\{F,G\} = \int_{\mathbb{D}_0} d^3a \left[\frac{\delta F}{\delta \zeta^\alpha(\vec{a})} \frac{\delta G}{\delta \pi_\alpha(\vec{a})} - \frac{\delta G}{\delta \zeta^\alpha(\vec{a})} \frac{\delta F}{\delta \pi_\alpha(\vec{a})} \right]$$

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

$$H[\zeta,\pi,s] = \int_{\mathbb{D}_0} \mathcal{H}(\zeta,\pi,s)\, d^3a, \quad \dot{\zeta}^\alpha = \{\zeta^\alpha, H\}, \quad \dot{\pi}_\beta = \{\pi_\beta, H\},$$

$$\dot{s} = \{s, H\} = 0$$

• **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:**

$$S[s] = \int_{\mathbb{D}_0} \rho_0(\vec{a})\, s(\vec{a},t)\, d^3a,$$

$$\{S,G\} = 0 \quad \forall \quad G$$

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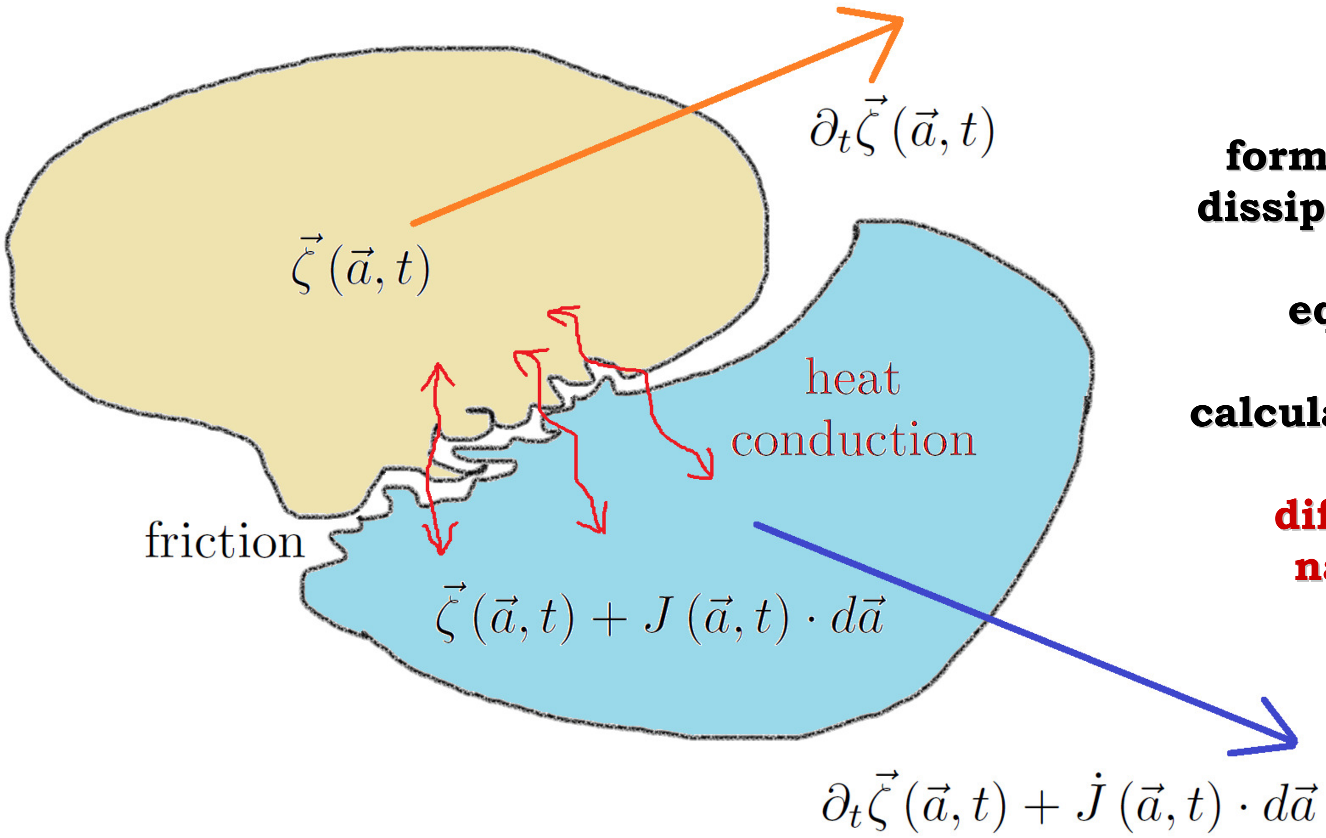
- **Lagrangian formalism in fluids and parcel variables: from the 6N particle variables to the 6 parcel centre-of-mass variables, plus entropy of the relative variables;**

- **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.**

- **Equations of motion of the non-ideal fluids in Lagrangian Formalism:**

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

$$\dot{\pi}^\alpha = -\frac{\partial}{\partial a^i}\left(pA^{\alpha i}\left(\partial\vec{\zeta}\right)\right) - \nabla^\alpha\phi + \mathcal{J}\left(\partial\vec{\zeta}\right)\nabla^\eta\sigma^\alpha{}_\eta,$$

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

$$\nabla^\alpha \stackrel{\text{def}}{=} \left(J^{-1}\right)^{\alpha i}\frac{\partial}{\partial a^i}, \quad \sigma_{\alpha\beta} = \Lambda_{\alpha\beta\gamma\delta}\left(J^{-1}\right)^{k\gamma}\frac{\partial\pi^\delta}{\partial a^k},$$

$$\Lambda_{\alpha\beta\gamma\delta} \stackrel{\text{def}}{=} \eta\left(\delta_{\delta\alpha}\delta_{\gamma\beta} + \delta_{\delta\beta}\delta_{\gamma\alpha} - \frac{2}{3}\delta_{\alpha\beta}\delta_{\gamma\delta}\right) + \zeta\delta_{\alpha\beta}\delta_{\gamma\delta}$$

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:

$$(F,G) =$$

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

$$\left. + \kappa T^2 \partial^k \left(\frac{1}{\rho T}\frac{\delta F}{\delta s} \right) \partial_k \left(\frac{1}{\rho T}\frac{\delta G}{\delta s} \right) \right\}$$

(ρ, s and v are the Eulerian variables mass density, mass-specific entropy density and bulk velocity).

OBTAINING THE RESULT

- **Correspondence between Eulerian and Lagrangian variables;**
- **Careful "dictionary" between the Frechet derivatives:**

$$\frac{\delta F}{\delta \varphi_L\left(\vec{a}\right)} = \mathcal{J}\left(\vec{a}\right)\frac{\delta F}{\delta \varphi_E\left(\vec{x}\right)} \quad / \quad \vec{\zeta}\left(\vec{a},t\right) = \vec{x}$$

This *caveat* renders it possible to write the metric bracket in Lagrangian Formalism as follows:

$$(F,G) =$$

$$= \frac{1}{\lambda}\int_{\mathbb{D}_0} \mathcal{J} d^3a \left\{ T\Lambda_{\alpha\beta\gamma\delta}\left[\nabla^\alpha\left(\frac{\delta F}{\delta \pi_\beta}\right) - \frac{1}{\rho_0 T}\nabla^\alpha\left(\frac{\pi^\beta}{\rho_0}\right)\frac{\delta F}{\delta s}\right]\left[\nabla^\gamma\left(\frac{\delta G}{\delta \pi_\delta}\right) - \frac{1}{\rho_0 T}\nabla^\gamma\left(\frac{\pi^\delta}{\rho_0}\right)\frac{\delta G}{\delta s}\right] + \right.$$

$$\left. + \kappa T^2 \nabla^\eta\left(\frac{1}{\rho_0 T}\frac{\delta F}{\delta s}\right)\nabla_\eta\left(\frac{1}{\rho_0 T}\frac{\delta G}{\delta s}\right)\right\}$$

Entropy generates the dissipative part of momentum and entropy-density dynamics through this metric bracket:

$$\left(\dot{\pi}_\eta\left(\vec{a}'\right)\right)_{\text{diss}} = \lambda\left(\pi_\eta\left(\vec{a}'\right), S\right), \quad \left(\dot{s}\left(\vec{a}'\right)\right)_{\text{diss}} = \lambda\left(s\left(\vec{a}'\right), S\right)$$

- **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 <<.,.>> is defined.**

$$\begin{cases} F = H + \lambda S, \\ H = \int_{\mathbb{D}_0} \left[\frac{\pi^2}{2\rho_0} + \rho_0 \phi\left(\vec{\zeta}\right) + \rho_0 \mathcal{U}\left(\frac{\rho_0}{\mathcal{J}}, s\right)\right] d^3a, \\ S[s] = \int_{\mathbb{D}_0} \rho_0\left(\vec{a}\right) s\left(\vec{a}, t\right) d^3a, \\ \dot{\Phi} = \langle\langle \Phi, F \rangle\rangle, \\ \langle\langle A, B \rangle\rangle = \{A, B\} + (A, B) \\ \{S, H\} = 0, \quad (S, H) = 0 \end{cases}$$

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** $\langle\langle A,B \rangle\rangle$ **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*;**

• **Introcing the parcel variables: ζ and π 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: ζ and π are involved in a symplecitc dynamics, while the entropy does not change at all, being a Casimir invariant;**

• **Non-ideal fluids: the formerly defind symplectic dynamics is enriched by a metric part, confering to π 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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