Contact geometry and thermodynamical systems

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Les Houches Summer Week: Joint Structures and Common Foundations of Statistical Physics, Information Geometry and Inference for Learning
July 27–31, 2020

[1] joint work with Manuel Laínz, David Martín de Diego and Alexandre Simões

In this paper, we introduce a differential geometric framework that incorporates in a very natural way fundamental thermodynamical concepts as the free energy and the rate of entropy production.
Typically, in the previous literature, this description needs to introduce appropriate Poisson and dissipation brackets with combined properties that allows the two laws of thermodynamics to be satisfied.
One of the most successful methods are based on the introduction of *metriplectic structures*:

Allan N. Kaufman. Dissipative Hamiltonian systems: a unifying principle. Phys. Lett. A, 100(8):419–422, 1984.
Philip J. Morrison. A paradigm for joined Hamiltonian and dissipative systems. volume 18, pages 410–419. 1986. Solitons and coherent structures (Santa Barbara, Calif., 1985).

coupling a Poisson and a gradient structure, where the entropy S is now constructed from a Casimir function of the Poisson structure.

Other approaches like in

B. J. Edwards and A. N. Beris. Noncanonical Poisson bracket for nonlinear elasticity with extensions to viscoelasticity. J. Phys. A, 24(11):2461–2480, 1991.
B. J. Edwards and A. N. Beris. Noncanonical Poisson bracket for nonlinear elasticity with extensions to viscoelasticity. J. Phys. A, 24(11):2461–2480, 1991.

use similar techniques, called *single generation formalism* introducing a generalized bracket which is naturally divided into two parts: a non-canonical Poisson bracket and a new dissipation bracket. The derived structures are capable of reproducing both reversible and irreversible evolutions providing a unifying formalism for many systems ruled by the laws of thermodynamics.

These approaches have proved to be very useful for the description of complex thermodynamical systems and also facilitate their numerical integration.

Recently, Gay-Balmaz and Yoshimura

F. Gay-Balmaz and H. Yoshimura. A Lagrangian variational formulation for nonequilibrium thermodynamics. Part I: Discrete systems. Journal of Geometry and Physics, 111:169–193, January 2017.
F. Gay-Balmaz and H. Yoshimura. From Lagrangian Mechanics to Nonequilibrium Thermodynamics: A Variational Perspective. Entropy, 21(1):8, January 2019.

have introduced a variational principle for the description of thermodynamical systems.

Their formulation extends the Hamilton principle of classical mechanics to include irreversible processes by introducing additional phenomenological and variational constraints.

A more geometrical approach is based on the use of contact geometry. In this approach, it is proposed that the thermodynamical phase space is equipped with a contact structure.

- Using the contact structure, it is possible to associate to each function f, a Hamiltonian vector field X_f which is the infinitesimal generator of a contact transformation.
- In this framework, the manifold of equilibrium states is represented by a Legendre submanifold N and the Hamiltonian vector field X_f is tangent to N if and only if the function f vanishes on N, that is, the Legendre submanifold is contained on the zero level set of the Hamiltonian function.
- The flow of X_f restricted to the Legendrian submanifold is interpreted as thermodynamical processes.

R. Mrugala, J. D. Nulton, J. Ch. Schon, and P. Salamon. Contact structure in thermodynamic theory. Reports on Mathematical Physics, 29(1):109–121, February 1991.

R. Mrugala. Continuous contact transformations in thermodynamics. In Proceedings of the XXV Symposium on Mathematical Physics (Torun, 1992), vol. 33, pages 149–154, 1993.

Another approach to the dynamics of thermodynamical processes is the one used in

R. Balian and P. Valentin. Hamiltonian structure of thermodynamics with gauge. The European Physical Journal B-Condensed Matter and Complex Systems, 21(2):269–282, 2001.
A. Van der Schaft and B. Maschke. Geometry of thermodynamic processes. Entropy, 20(12):925, 2018.

which is based on homogeneous symplectic Hamiltonian systems, and is completely equivalent to the contact Hamiltonian vector field approach.

More recently, there has been a resurgence of interest in the study of contact dynamics, mainly for the applications in the study of dissipative systems and their geometric properties. We will reviews some of that results and their applications to thermodynamical systems.

Outline of the talk

1. Contact geometry and contact dynamics
2. Jacobi and Cartan brackets
3. Mechanical systems
4. Simple mechanical systems with friction
5. Linearly damped systems
6. Discrete Herglotz equations
7. Conclusions and future work

Contact geometry and contact dynamics

We will consider some ingredients of contact geometry that we will need in the sequel.
Let M be a differentiable manifold of dimension $2n+1$ and a 1-form η on M. We say that η is a contact 1-form if $\eta \wedge (d\eta)^n \neq 0$ at every point. Then, we call (M, η) a contact manifold. A distinguished vector field for a contact manifold is the Reeb vector field $R \in \mathfrak{X}(M)$ univocally characterized by

$$i_R \eta = 1 \quad \text{and} \quad i_R d\eta = 0 \, .$$

We can define also an isomorphism of $C^\infty(M, \mathbb{R})$ modules by

$$\begin{array}{rccc} \flat : & \mathfrak{X}(M) & \longrightarrow & \Omega^1(M) \\ & X & \longmapsto & i_X d\eta + \eta(X)\eta \end{array}$$

Observe that $\flat^{-1}(\eta) = R$.

Using the generalized Darboux theorem, we have canonical coordinates (q^i, p_i, S), $1 \leq i \leq n$ in a neighborhooh of every point $x \in M$, such that the contact 1-form η and the Reeb vector field are:

$$\eta = dS - p_i \, dq^i \qquad \text{and} \qquad R = \frac{\partial}{\partial S} \, .$$

Define the bi-vector Λ on M by

$$\Lambda(\alpha, \beta) = -d\eta(\flat^{-1}(\alpha), \flat^{-1}(\beta)), \qquad \alpha, \beta \in \Omega^1(M) \, . \tag{1}$$

In canonical coordinates,

$$\Lambda = \frac{\partial}{\partial p_i} \wedge \left(\frac{\partial}{\partial q^i} + p_i \frac{\partial}{\partial S} \right) \tag{2}$$

Define the $C^\infty(M, \mathbb{R})$-linear mapping

$$\sharp_\Lambda : \Omega^1(M) \to \mathfrak{X}(M)$$

by $\langle \beta, \sharp(\alpha) \rangle = \Lambda(\alpha, \beta)$ with $\alpha, \beta \in \Omega^1(M)$.

Given a function $f \in C^\infty(M, \mathbb{R})$ we will define the following vector fields

- **Hamiltonian or contact vector field** X_f defined by

$$X_f = \sharp_\Lambda(df) - fR$$

or in other terms, X_f is the unique vector field such that

$$\flat(X_f) = df - (R(f) + f)\,\eta\ .$$

In canonical coordinates:

$$X_f = \frac{\partial f}{\partial p_i}\frac{\partial}{\partial q^i} - \left(\frac{\partial f}{\partial q^i} + p_i\frac{\partial f}{\partial S}\right)\frac{\partial}{\partial p_i} + \left(p_i\frac{\partial f}{\partial p_i} - f\right)\frac{\partial}{\partial S}$$

- **The evolution or horizontal vector field**

$$\mathcal{E}_f = \sharp_\Lambda(df) = X_f + fR$$

or

$$\flat(\mathcal{E}_f) = df - R(f)\,\eta\ .$$

In canonical coordinates:

$$\mathcal{E}_f = \frac{\partial f}{\partial p_i}\frac{\partial}{\partial q^i} - \left(\frac{\partial f}{\partial q^i} + p_i\frac{\partial f}{\partial S}\right)\frac{\partial}{\partial p_i} + p_i\frac{\partial f}{\partial p_i}\frac{\partial}{\partial S}$$

Remarks

1. We will see that the evolution vector field will be useful to describe some simple isolated thermodynamical systems with friction, where the variable S will play the role of the entropy of the system.
2. The interpretation of the variable S as being the entropy of the system excludes the possibility of using cosymplectic geometry to describe thermodynamical systems. Indeed, if the thermodynamical equations were the integral curves of the cosymplectic Hamiltonian vector field, then the entropy production would be constant, which is not the general situation.

Jacobi and Cartan brackets

The pair $(\Lambda, E = -R)$ is a particular case of Jacobi structure since it satisfies

$$[\Lambda, \Lambda] = 2E \wedge \Lambda \quad \text{and} \quad [\Lambda, E] = 0 \ .$$

From this Jacobi structure we can define the Jacobi bracket as follows:

$$\{f, g\} = \Lambda(df, dg) + fE(g) - gE(f), \quad f, g \in C^\infty(M, \mathbb{R})$$

The mapping $\{\ ,\ \} : C^\infty(M, \mathbb{R}) \times C^\infty(M, \mathbb{R}) \longrightarrow C^\infty(M, \mathbb{R})$ is bilinear, skew-symmetric and satisfies the Jacobi's identity but, in general, it does not satisfy the Leibniz rule; this last property is replaced by a weaker condition:

$$\text{Supp}\ \{f, g\} \subset \text{Supp}\ f \cap \text{Supp}\ g \ .$$

In this sense, this bracket generalizes the well-known Poisson brackets. Indeed, a Poisson manifold is a particular case of Jacobi manifold. In local coordinates

$$\{f, g\} \quad = \quad \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} - \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial S}\left(p_i\frac{\partial g}{\partial p_i} - g\right) + \frac{\partial g}{\partial S}\left(p_i\frac{\partial f}{\partial p_i} - f\right)$$

It is also interesting for us to introduce the bracket (*Cartan bracket*) that does not obey the Jacobi identity

$$
\begin{aligned}
[f, g] &= \Lambda(df, dg) \\
&= \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} - \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial S}\left(p_i \frac{\partial g}{\partial p_i}\right) + \frac{\partial g}{\partial S}\left(p_i \frac{\partial f}{\partial p_i}\right)
\end{aligned}
$$

Mechanics

Our main example of contact manifold along this talk will be $T^*Q \times \mathbb{R}$, where Q is n-dimensional manifold, with contact structure defined by

$$\eta = pr_2^*(dS) - pr_1^*(\theta_Q) \equiv dS - \theta_Q$$

where $pr_1 : T^*Q \times \mathbb{R} \to T^*Q$ and $pr_2 : T^*Q \times \mathbb{R} \to \mathbb{R}$ are the canonical projections and θ_Q is the Liouville 1-form on the cotangent bundle defined by

$$\Theta_Q(X_{\mu_q}) = \langle \mu_q, T_{\mu_q}\pi_Q X_{\mu_q} \rangle$$

being $X_{\mu_q} \in T_{\mu_q}T^*Q$. Taking bundle coordinates (q^i, p_i) on T^*Q we have that $\eta = dS - p_i dq^i$.

On such a manifold we can define the bi-vector

$$\Lambda_0 = \Lambda + \sharp_\Lambda(dS) \wedge R$$

which is Poisson, that is $[\Lambda_0, \Lambda_0] = 0$. In coordinates,

$$\Lambda_0 = \frac{\partial}{\partial p_i} \wedge \frac{\partial}{\partial q^i}$$

is like the canonical Poisson bracket on T^*Q but now applied to functions on $T^*Q \times \mathbb{R}$.

Observe that in this case the Cartan bracket can be rewritten in terms of the Poisson bracket induced by Λ_0 and an extra term that describe the thermodynamical behaviour. That is,

$$[f, g] = \{f, g\}_{\Lambda_0} - \frac{\partial f}{\partial S}\Delta g + \frac{\partial g}{\partial S}\Delta f$$

where $\Delta = -\sharp_\Lambda(dS)$ is the Liouville vector field:

$$\Delta = p_i \frac{\partial}{\partial p_i}$$

We will denote by

$$\{f, g\}_\Delta = \frac{\partial g}{\partial S}\Delta f - \frac{\partial f}{\partial S}\Delta g$$

then the Cartan bracket is written as in the single generation formalism as

$$[f, g] = \{f, g\}_{\Lambda_0} + \{f, g\}_\Delta \tag{3}$$

Now, we will discuss some interesting properties of the qualitative behaviour of the evolution vector field $\mathcal{E}_f$.

Proposition The Lie derivative of the contact form η with respect to the evolution vector field $\mathcal{E}_f$ associated to the Hamiltonian function f satisfies the following relation

$$\mathcal{L}_{\mathcal{E}_f}\eta = -R(f)\eta + df \ .$$

Proof:
The proof is a trivial consequence of the properties of the Lie derivative and the properties of the Hamiltonian vector field:

$$\begin{aligned} \mathcal{L}_{\mathcal{E}_f}\eta &= \mathcal{L}_{X_f+fR}\eta = \mathcal{L}_{X_f}\eta + \mathcal{L}_{fR}\eta \\ &= -R(f)\eta + (i_R\eta)df = -R(f)\eta + df \end{aligned}$$

Theorem

Let $\mathcal{L}_c(f) = f^{-1}(c)$ be a level set of $f : M \to \mathbb{R}$ where $c \in \mathbb{R}$. We assume that $\mathcal{L}_c(f) \neq 0$ and $R(f)(x) \neq 0$ for all $x \in \mathcal{L}_c(f)$. Then

1. *The 2-form $\omega_c \in \Omega^2(\mathcal{L}_c(f))$ defined by*

$$\omega_c = -di_c^*\eta$$

   is an exact symplectic structure. Here $i_c : \mathcal{L}_c f \hookrightarrow M$ denotes the canonical inclusion

2. *If Δ_c is the Liouville vector field, that is,*

$$i_{\Delta_c}\omega_c = i_c^*\eta$$

   then the restriction of $\mathcal{E}_f$ to $\mathcal{L}_c(f)$ verifies that

$$\mathcal{E}_f\big|_{\mathcal{L}_c(f)} = R(f)\big|_{\mathcal{L}_c(f)}\Delta_c$$

Proof:
The form ω_c is trivially closed. To see that it is a symplectic form, we just need to check that is non degenerate. Let $p \in \mathcal{L}_c(f)$. Notice that, at that point, $\omega_c = -d\eta|_{T_p\mathcal{L}_c(f)}$. By the condition $R(f) \neq 0$, we have that R_p (and, hence $\ker \eta = \text{span}\langle R \rangle$) is transverse to $T_p\mathcal{L}_c(f)$. But since $\eta_p \wedge d\eta_p^n \neq 0$,then $d\eta|_V$ is non-degenerate for every subspace V transverse to $\ker \eta$. Therefore, ω_c is also non-degenerated.
For the second part, we first remark that $\mathcal{E}_f(f) = 0$, hence $(i_c)_*\mathcal{E}_f = \mathcal{E}_f|_{\mathcal{L}_c(f)}$ is a well-defined vector field. By the above Proposition and Cartan's identity

$$i_{\mathcal{E}_f} d\eta = -R(f)\eta + df.$$

Pulling back by i_c, we get

$$i_{(i_c)_*\mathcal{E}_f} i_c^* d\eta = -(R(f) \circ i_c) i_c^* \eta + d i_c^* f = -(R(f) \circ i_c) i_c^* \eta,$$

dividing by $-(R(f) \circ i_c)$,

$$-i_{(i_c)_*\mathcal{E}_f/R(f)} i_c^* d\eta = i_{(i_c)_*\mathcal{E}_f/R(f)} \omega_c = i_c^* \eta.$$

Thus, $(i_c)_* (\mathcal{E}_f/R(f)) = \Delta_c$, as we wanted to show.

Remarks

1. Observe that since

$$\mathcal{E}_f\big|_{\mathcal{L}_c(f)} = R(f)\big|_{\mathcal{L}_c(f)}\Delta_c$$

then the dynamics on each energy level is like a Liouville dynamics after a time reparametrization

$$dt = \frac{1}{R(f)} d\tau \ .$$

2. It is interesting to note that $T^*Q \times \mathbb{R}$ is also the phase space for time-dependent dynamics. In this case, the appropriate formalism is the cosymplectic formalism where the canonical cosymplectic structure is given by (dt, ω_Q)

A. Bravetti, M. de León, J. C. Marrero, E. Padrón: Invariant measures for contact Hamiltonian systems: symplectic sandwiches with contact bread arXiv:2006.15123

- We prove that, under some natural conditions, Hamiltonian systems on a contact manifold C can be split into a Reeb dynamics on an open subset of C and a Liouville dynamics on a submanifold of C of codimension 1.
- For the Reeb dynamics we find an invariant measure.
- Moreover, we show that, under certain completeness conditions, the existence of an invariant measure for the Liouville dynamics can be characterized using the notion of a symplectic sandwich with contact bread.

Simple mechanical systems with friction

We will use the evolution vector field to describe simple thermodynamical systems, that is, thermodynamical systems whose configuration space is composed by just one scalar thermal variable (in our case the entropy) and a finite set of mechanical variables (position and momenta). We will assume that the system is isolated, that is, there is not any transfer of work, matter or heat.

The isolated simple thermodynamical systems are described by a Lagrangian function:

$$\begin{array}{rccc} L: & TQ \times \mathbb{R} & \longrightarrow & \mathbb{R} \\ & (v_q, S) & \longmapsto & L(v_q, S) \end{array}$$

where Q is the configuration manifold describing the mechanical part of the thermodynamical system, TQ is the tangent bundle with canonical projection $\tau_Q : TQ \to Q$ given by $\tau_Q(v_q) = q$. The entropy of the system is described by the real variable $S \in \mathbb{R}$. If we consider coordinates (q^i) on Q and induced coordinates $(q^i, \dot{q}^i)$ on TQ, then $\tau_Q(q^i, \dot{q}^i) = (q^i)$.

We will see that the Lagrangian function itself will produce a friction force satisfying naturally the two laws of thermodynamics.

We will assume that the Lagrangian system is regular, that is, the matrix

$$(W_{ij}) = \left(\frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \right)$$

is regular or, equivalently, the mapping $\mathbb{F}L : TQ \times \mathbb{R} \to T^*Q \times \mathbb{R}$ is a local diffeomorphism, where:

$$\mathbb{F}L(q^i, \dot{q}^i, S) = \left(q^i, \frac{\partial L}{\partial \dot{q}^i}, S \right)$$

is the Legendre transform. For simplicity, we will assume that the Legendre transform is a global diffeomorphism, since if it was only a local diffeomorphism we could proceed analogously by restricting to a neighbourhood. Then, we may define a Hamiltonian function $H : T^*Q \times \mathbb{R} \to \mathbb{R}$ given by

$$H(q^i, p_i, S) = p_i \dot{q}^i - L(q^i, \dot{q}^i, S)$$

where now the coordinates $\dot{q}^i$ are implicitly defined by the relations $p_j = \frac{\partial L}{\partial \dot{q}^j}(q^i, \dot{q}^i, S)$.

The equations of motion defined by the evolution vector field $\mathcal{E}_H$ are

$$\begin{aligned} \frac{dq^i}{dt} &= \frac{\partial H}{\partial p_i}\,, \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial p_i} - p_i\frac{\partial H}{\partial S} \\ \frac{dS}{dt} &= p_i\frac{\partial H}{\partial p_i}\,. \end{aligned}$$

The vector field $\mathcal{E}_H$ satisfies the following two properties that correspond to the first and second laws of thermodynamics: conservation of the energy of an isolated system and irreversibility of the processes, that is, non-decreasing entropy production.

Proposition The integral curves of $\mathcal{E}_H$ satisfies the following properties:

1. $\mathcal{E}_H(H) = 0$, that is, $\frac{dH}{dt} = 0$;
2. $\mathcal{E}_H(S) = \Delta(H)$, that is, $\frac{dS}{dt} = \Delta H$.

Proof Both are a direct consequence of the definition of the evolution vector field $\mathcal{E}_H = \sharp_\Lambda(dH)$.

Assume that the Hamiltonian H is given by

$$H(q^i, p_i, S) = \frac{1}{2} g^{ij} p_i p_j + V(q, S) \quad (4)$$

where (g^{ij}) is positive semi-definite (for instance, it is associated to a Riemannian metric on Q). Then, the vector field $\mathcal{E}_H$ describes an isolated simple thermodynamical system with friction satisfying the first and second laws of thermodynamics:

Proposition The integral curves of $\mathcal{E}_H$ satisfies the following properties:

1. **First law of Thermodynamics**:

$$\frac{dH}{dt} = 0 \quad \text{(preservation of the total energy);}$$

2. **Second law of Thermodynamics**:

$$\frac{dS}{dt} = \Delta H \geq 0 \quad \text{(total entropy of an isolated system never decreases).}$$

Proof It is a direct consequence of the above Proposition and $\Delta H = p_i g^{ij} p_j \geq 0$.

If we express the dynamics in terms of the brackets defined in (3) we have that

$$\dot{f} = \{f, H\}_{T^*Q} + \{f, H\}_{\Delta}. \tag{5}$$

Obviously,

$\{H, H\}_{T^*Q} = \{H, H\}_{\Delta} = 0$ (first law)

and

$\{S, H\}_{T^*Q} = 0$ and $\{S, H\}_{\Delta} = \Delta H \geq 0$ (second law).

Observe that in Equation (5) both brackets are using the function H as "generator". This is the reason that typically this formalism is known as *single generator formalism*.

Linearly damped systems

Consider a linearly damped system described by coordinates (q, p, S), where q represents the position, p the momentum of the particle and S is the entropy of the surrounding thermal bath. We assume that the system is subjected to a viscous friction force, proportional to the minus velocity of the particle. The system is described by the Hamiltonian

$$H(q, p, S) = \frac{p^2}{2m} + V(q) + \gamma S, \quad \gamma > 0.$$

Therefore, the equations of motion for $\mathcal{E}_H = \sharp_\Lambda(dH)$ are:

$$\begin{pmatrix} \dot{q} \\ \dot{p} \\ \dot{S} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & -p \\ 0 & p & 0 \end{pmatrix} \begin{pmatrix} V'(q) \\ p/m \\ \gamma \end{pmatrix}$$

or

$$\begin{aligned} \dot{q} &= \frac{p}{m} \\ \dot{p} &= -V'(q) - \gamma p \\ \dot{S} &= \frac{p^2}{m} \end{aligned}$$

In the Lagrangian side we obtain the system given by

$$\begin{aligned} m\ddot{q} &= -V'(q) - \gamma m\dot{q} \\ \dot{S} &= m\dot{q}^2. \end{aligned}$$

Observe that in this system the friction force is given by the map $F_{fr} : TQ \to T^*Q$ given by

$$F_{fr}(q, \dot{q}) = \gamma \dot{q}^i dq^i.$$

Therefore, the equation of entropy production can be rewritten in terms of the friction force as follows

$$T\dot{S} = -\langle F_{fr}(q, \dot{q}), \dot{q} \rangle$$

where $T = \frac{\partial H}{\partial S} = -\frac{\partial L}{\partial S} = \gamma > 0$ represents the temperature of the thermal bath. These equations coincide with the set of equations proposed by Gay-Balmaz and Yoshimura for this particular choice of Lagrangian L and friction force F_{fr}. Observe that, in this particular example where the temperature satisfies $T = \gamma$, the equations are only defined for values $\gamma > 0$ and thus we are only modelling thermodynamical systems with non-zero temperature.

Observe that the two brackets are:

$$\begin{aligned}
\{f,g\}_{\Lambda_0} &= \frac{\partial f}{\partial p}\frac{\partial g}{\partial q} - \frac{\partial g}{\partial p}\frac{\partial f}{\partial q} \\
\{f,g\}_{\Delta} &= p\frac{\partial g}{\partial S}\frac{\partial f}{\partial p} - p\frac{\partial f}{\partial S}\frac{\partial g}{\partial p}
\end{aligned}$$

In particular

$$\begin{aligned}
\{H,g\}_{\Lambda_0} &= \frac{p}{m}\frac{\partial g}{\partial q} - \frac{\partial g}{\partial p}V'(q) \\
\{H,g\}_{\Delta} &= \frac{p^2}{m}\frac{\partial g}{\partial S} - \gamma p\frac{\partial g}{\partial p}
\end{aligned}$$

and

$$\mathcal{E}_H(g) = \dot{g} = \{H,g\}_{\Lambda_0} + \{H,g\}_{\Delta}$$

Therefore it is clear that $\{H,H\}_{\Lambda_0} = 0$ and $\{H,H\}_{\Delta} = 0$ (by skew-symmetry) and $\{H,S\}_{\Lambda_0} = 0$ and $\{H,S\}_{\Delta} = \frac{p^2}{m} \geq 0$.

The geometric setting

Let $L : TQ \times \mathbb{R} \longrightarrow \mathbb{R}$ be a regular Lagrangian function, and introduce coordinates on $TQ \times \mathbb{R}$, denoted by $(q^i, \dot{q}^i, S)$, where (q^i) are coordinates in Q, $(q^i, \dot{q}^i)$ are the induced bundle coordinates in TQ and S is a global coordinate in $\mathbb{R}$. Using the canonical endomorphism $\mathbf{S}$ on TQ locally defined by

$$\mathbf{S} = dq^i \otimes \frac{\partial}{\partial \dot{q}^i},$$

one can construct a 1-form λ_L on $TQ \times \mathbb{R}$ given by

$$\lambda_L = \mathbf{S}^*(dL)$$

where now $\mathbf{S}$ and $\mathbf{S}^*$ are the natural extensions of $\mathbf{S}$ and its adjoint operator $\mathbf{S}^*$ to $TQ \times \mathbb{R}$. Therefore, we have that

$$\lambda_L = \frac{\partial L}{\partial \dot{q}^i}\, dq^i.$$

M. de León and M. Lainz. Singular lagrangians and precontact hamiltonian systems . International Journal of Geometric Methods in Modern Physics, 2019.

M. de León and M. Lainz. Infinitesimal symmetries in contact hamiltonian systems. Journal of Geometry and Physics, 2020.

Now, the 1-form on $TQ \times \mathbb{R}$ given by $\eta_L = dS - \lambda_L$ or, in local coordinates, by

$$\eta_L = dS - \frac{\partial L}{\partial \dot{q}^i}\, dq^i$$

is a contact form on $TQ \times \mathbb{R}$ if and only if L is regular; indeed, if L is regular, then we may prove that $\eta_L \wedge (d\eta_L)^n \neq 0$, and the converse is also true.

The corresponding Reeb vector field is given in local coordinates by

$$\mathcal{R}_L = \frac{\partial}{\partial S} - W^{ij} \frac{\partial^2 L}{\partial \dot{q}^j \partial S}\, \frac{\partial}{\partial \dot{q}^i},$$

where (W^{ij}) is the inverse matrix of the Hessian (W_{ij}).

The energy of the system is defined by

$$E_L = \Delta(L) - L$$

where $\Delta = \dot{q}^i \, \frac{\partial}{\partial \dot{q}^i}$ is the natural extension of the Liouville vector field on TQ to $TQ \times \mathbb{R}$. Therefore, in local coordinates we have that

$$E_L = \dot{q}^i \, \frac{\partial L}{\partial \dot{q}^i} - L$$

Denote by $\flat_L : T(TQ \times \mathbb{R}) \longrightarrow T^*(TQ \times \mathbb{R})$ the vector bundle isomorphism given by

$$\flat_L(v) = i_v(d\eta_L) + (i_v\eta_L)\,\eta_L$$

where η_L is the contact form on $TQ \times \mathbb{R}$ previously defined. We shall denote its inverse isomorphism by $\sharp_L = (\flat_L)^{-1}$.
Let ξ_L be the unique vector field satisfying the equation

$$\flat_L(\xi_L) = dE_L - (\mathcal{R}_L E_L + E_L)\,\eta_L. \tag{6}$$

A direct computation from eq. (6) shows that if $(q^i(t), \dot{q}^i(t), S(t))$ is an integral curve of ξ_L, then it satisfies the generalized Euler-Lagrange equations considered by G. Herglotz in 1930:

$$\begin{aligned} &\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = \frac{\partial L}{\partial \dot{q}^i}\frac{\partial L}{\partial S}\ , \\ &\dot{S} = L(q^i, \dot{q}^i, S)\ . \end{aligned} \tag{7}$$

Now, given a regular Lagrangian function L, we may define the bi-vector Λ_L on $TQ \times \mathbb{R}$ as in (1) associated to the contact form η_L. That is,

$$\Lambda_L(\alpha, \beta) = -d\eta_L(\flat_L^{-1}(\alpha), \flat_L^{-1}(\beta)), \qquad \alpha, \beta \in \Omega^1(TQ \times \mathbb{R})\ . \tag{8}$$

If $(q^i(t), \dot{q}^i(t), S(t))$ is an integral curve of the evolution vector field $\mathcal{E}_L$ associated to the contact form η_L defined by

$$\mathcal{E}_L = \sharp_{\Lambda_L}(dE_L) \text{ or } \flat_L(\xi_L) = dE_L - (\mathcal{R}_L E_L)\,\eta_L\ ,$$

then it satisfies the thermodynamical Herglotz equations

$$\begin{aligned} &\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i} = \frac{\partial L}{\partial \dot{q}^i}\frac{\partial L}{\partial S}. \\ &\dot{S} = \dot{q}^i \frac{\partial L}{\partial \dot{q}^i}. \end{aligned} \tag{9}$$

Moreover, if H is the Hamiltonian function defined by $H = E_L \circ (\mathbb{F}L)^{-1}$, where $\mathbb{F}L : TQ \times \mathbb{R} \to T^*Q \times \mathbb{R}$ is the Legendre transform, then the evolution vector field $\mathcal{E}_H$ associated to H is $\mathbb{F}L$-related to $\mathcal{E}_L$.

Variational formulation of contact Lagrangian mechanics

Let $L : TQ \times \mathbb{R} \to \mathbb{R}$ be a Lagrangian function. In this section we will recall the so-called Herglotz's principle, a modification of Hamilton's principle that allows us to obtain Herglotz's equations, sometimes called generalized Euler-Lagrange equations.
Fix $q_1, q_2 \in Q$ and an interval $[a, b] \subset \mathbb{R}$. We denote by $\Omega(q_1, q_2, [a, b]) \subseteq (\mathcal{C}^\infty([a, b] \to Q))$ the space of smooth curves ξ such that $\xi(a) = q_1$ and $\xi(b) = q_2$. This space has the structure of an infinite dimensional smooth manifold whose tangent space at ξ is given by the set of vector fields over ξ that vanish at the endpoints, that is,

$$\begin{aligned} T_\xi \Omega(q_1, q_2, [a, b]) = \{ v_\xi \in \mathcal{C}^\infty([a, b] \to TQ) \mid \\ \tau_Q \circ v_\xi = \xi,\ v_\xi(a) = 0,\ v_\xi(b) = 0 \}. \end{aligned} \tag{10}$$

We will consider the following maps. Fix $c \in \mathbb{R}$. Let

$$\mathcal{Z} : \Omega(q_1, q_2, [a, b]) \to \mathcal{C}^\infty([a, b] \to \mathbb{R}) \tag{11}$$

be the operator that assigns to each curve ξ the curve $\mathcal{Z}(\xi)$ that solves the following ODE:

$$\frac{d\mathcal{Z}(\xi)(t)}{dt} = L(\xi(t), \dot{\xi}(t), \mathcal{Z}(\xi)(t)), \quad \mathcal{Z}(\xi)(a) = c. \tag{12}$$

Now we define the *action functional* as the map which assigns to each curve the solution to the previous ODE evaluated at the endpoint:

$$\begin{aligned} \mathcal{A} : \Omega(q_1, q_2, [a, b]) &\to \mathbb{R}, \\ \xi &\mapsto \mathcal{Z}(\xi)(b), \end{aligned} \tag{13}$$

that is, $\mathcal{A} = ev_b \mathcal{Z}$, where $ev_b : \zeta \mapsto \zeta(b)$ is the evaluation map at b.

Theorem

(Contact variational principle) Let $L : TQ \times \mathbb{R} \to \mathbb{R}$ *be a Lagrangian function and let* $\xi \in \Omega(q_1, q_2, [a, b])$ *be a curve in* Q*. Then,* $(\xi, \dot{\xi}, \mathcal{Z}(\xi))$ *satisfies the Herglotz's equations if and only if* ξ *is a critical point of* $\mathcal{A}$*.*

This theorem generalizes Hamilton's Variational Principle. In the case that the Lagrangian is independent of the $\mathbb{R}$ coordinate (i.e., $L(x, y, z) = \hat{L}(x, y)$) the contact Lagrange equations reduce to the usual Euler-Lagrange equations. In this situation, we can integrate the ODE of (13) and we get

$$\mathcal{A}(\xi) = \int_a^b \hat{L}(\xi(t), \dot{\xi}(t))t + \frac{c}{b-a}, \tag{14}$$

that is, the usual Euler-Lagrange action up to a constant.

Discrete Herglotz equations

Now, we propose to construct a numerical integrator for $\mathcal{E}_L$ based on a similar method to the discrete Herglotz principle.
Let $L_d : Q \times Q \times \mathbb{R} \to \mathbb{R}$ be a discrete Lagrangian function. Then a possible integrator for the evolution dynamics is

$$D_1 L_d(q_1, q_2, S_1) + (1 + D_S L_d((q_1, q_2, S_1))D_2 L_d(q_0, q_1, S_0) = 0 \quad (15)$$

and the entropy is subjected to

$$S_1 - S_0 = (q_1 - q_0) D_2 L_d(q_0, q_1, S_0). \quad (16)$$

M. Vermeeren, A. Bravetti, and M. Seri. Contact variational integrators. J. Phys. A, 52(44):445206, 28, 2019.
A. Simoes, M. de León, M. Lainz, and D. Martín de Diego. On the geometry of discrete contact mechanics. arxiv:2003.11892 [math.ph], 2020.

Example Consider again the Hamiltonian function of the damped harmonic oscillator. Since H is regular, we may consider the corresponding Lagrangian function $L : TQ \times \mathbb{R} \to \mathbb{R}$ given by

$$L(q, \dot{q}, S) = \frac{\dot{q}^2}{2} - \frac{q^2}{2} - \gamma S.$$

A standard discretization of this Lagrangian function is given by means of a quadrature rule like

$$L_d(q_0, q_1, S_0) = \frac{(q_1 - q_0)^2}{2h} - h\frac{(q_1 + q_0)^2}{8} - h\gamma S_0.$$

The discrete Herglotz equations (15) together with (16) give the explicit integrator

$$\begin{aligned} q_2 &= \frac{\gamma h^3 q_0 + \gamma h^3 q_1 + 4\gamma h q_0 - 4\gamma h q_1 - h^2 q_0 - 2h^2 q_1 - 4q_0 + 8q_1}{h^2 + 4} \\ S_1 &= S_0 + \frac{(q_1 - q_0)^2}{h} - h\frac{q_1^2 - q_0^2}{4}. \end{aligned} \tag{17}$$

In Figure 1 we plot the integrator given by equations (17). We see that the qualitative behaviour of the integrator is also quite good. In fact, an open question is whether the error can be improved by considering discrete Lagrangian functions approximating well enough the exact discrete Lagrangian function.

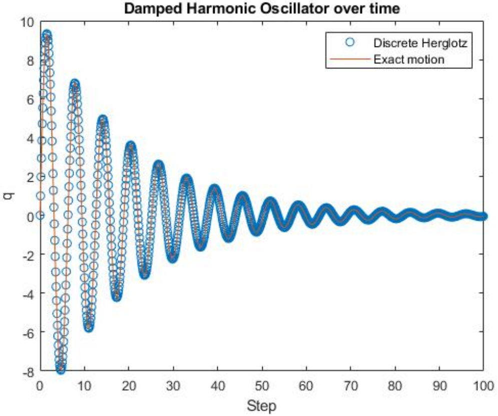

Figure: Trajectory of (17): the initial data are $q_0 = 0$, $q_1 = 1$ and $S_0 = 0$; the step is $h = 0.1$ and $\gamma = 0.1$. We plot the positions q_k and compare the integrator with the integral curve of the evolution dynamics $\mathcal{E}_L$.

As a last comment, the entropy for equations (17) is increasing and the Hamiltonian oscillates before stabilizing around a constant value (cf. Fig 2).

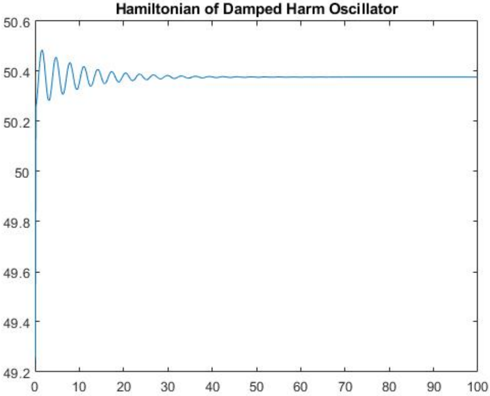

Figure: Hamiltonian of (17): using the same initial data and settings from Figure 1, we plot the Hamiltonian function along the iterations of the integrator.

Conclusions and future work

- We have shown the importance of the evolution or horizontal vector field to describe simple thermodynamical systems.
- We have proven that the restriction of this vector field to constant energy hypersurfaces is a time reparametrization of a Liouville vector field.
- Also, the relation with the single generation formalism is elucidated and the construction of geometric integrators satisfying the two laws of thermodynamics.
- Moreover, we will study the possibility of introducing the techniques developed in discrete mechanics, in particular, variational integrators, to numerically integrate the equations of the evolution vector field associated to a given Lagrangian function $L : TQ \times \mathbb{R} \longrightarrow \mathbb{R}$.
- This would allow us to develop higher order methods in a simple way. In recent papers a discrete Herglotz principle has been introduced, allowing to obtain integrators for Lagrangian contact systems. We think that it is possible to adapt the previous constructions to the case of evolution vector fields.

- Of course, the techniques developed in this paper were applied to simple thermodynamical systems but we consider them to be the building blocks to model more evolved thermodynamical systems using interconnection of these simple systems or working with other types of Jacobi manifolds.
- In our paper, we have initially started with contact structures but the proposed framework is also valid for general Jacobi manifolds which naturally cover other interesting examples of thermodynamical systems. As an example, consider a Poisson manifold (M, Λ), that is, a differentiable manifold M equipped with a bivector field Λ with associated bracket $\{\ ,\ \}$ verifying that $[\Lambda, \Lambda] = 0$. Let $k \in C^\infty(M)$ and consider the corresponding Hamiltonian vector field with respect to this Poisson structure

$$X_k = \Lambda(\cdot, dk) = \sharp_\Lambda(dk)$$

Define the conformal Poisson tensor (with conformal factor k) $\Lambda_k = k\Lambda$. Then (Λ_k, X_k) is a Jacobi manifold. In other words,

$$[\Lambda_k, \Lambda_k] = 2X_k \wedge \Lambda_k, \qquad [X_k, \Lambda_k] = 0.$$

This structure appears, for instance, on a model with heat exchange between different subsystems.

As a simple example, consider two simple thermodynamical subsystems (for instance, two ideal gases)
H. Ramírez, B. Maschke, and D. Sbarbaro. Modelling and control of multi-energy systems: an irreversible port-Hamiltonian approach. Eur. J. Control, 19(6):513–520, 2013.
which may interact through a conducting wall. The variables are (S_1, S_2), representing the entropies of subsystem 1 and 2, respectively. Suppose that the Hamiltonian function is of the form

$$H(S_1, S_2) = U(S_1) + U(S_2),$$

where $U(S_i)$ represents the internal energy of each subsystem and consider the function

$$k(S_1, S_2) = \lambda \left(\frac{1}{\frac{\partial U}{\partial S_1}} - \frac{1}{\frac{\partial U}{\partial S_2}} \right) = \lambda \left(\frac{1}{T_1} - \frac{1}{T_2} \right)$$

where $\lambda > 0$ is the Fourier heat conduction coefficient and $T_i = \frac{\partial U}{\partial S_i} > 0$, $i = 1, 2$, represents the temperature of each subsystem.

Taking the canonical Poisson structure on $\mathbf{R}^2$

$$\Lambda = \frac{\partial}{\partial S_1} \wedge \frac{\partial}{\partial S_2} \ ,$$

consider the associated Jacobi manifold (Λ_k, X_k) and the corresponding evolution vector field $\mathcal{E}_H$:

$$\begin{aligned}
\mathcal{E}_H &= \sharp_{\Lambda_k}(dH) = \lambda \left(\frac{\frac{\partial U}{\partial S_2}}{\frac{\partial U}{\partial S_1}} - 1 \right) \frac{\partial}{\partial S_1} - \lambda \left(1 - \frac{\frac{\partial U}{\partial S_1}}{\frac{\partial U}{\partial S_2}} \right) \frac{\partial}{\partial S_2} \\
&= \lambda \left(\frac{T_2}{T_1} - 1 \right) \frac{\partial}{\partial S_1} + \lambda \left(\frac{T_1}{T_2} - 1 \right) \frac{\partial}{\partial S_2}
\end{aligned}$$

Obviously $\mathcal{E}_H(H) = 0$ and moreover, considering the total entropy $S = S_1 + S_2$

$$\mathcal{E}_H(S_1 + S_2) = \frac{\lambda}{T_1 T_2} \left(T_2^2 - 2 T_1 T_2 + T_1^2 \right) = \frac{\lambda}{T_1 T_2} (T_2 - T_1)^2 \geq 0 \ .$$

It is interesting to study the qualitative geometric properties induced by different Jacobi structures for the study of systems that couple mechanical and thermodynamical behaviour.

- Another interesting subject to study consists on applying our theory to other Jacobi manifolds derived by symmetry reduction. For instance, we can start with a contact structure on $T^*G \times \mathbb{R}$ where G is a Lie group and assuming invariance under left (or right) translation of the Hamiltonian function, we obtain a reduced system with dissipation (for instance, rigid body equations with linear dissipation defined on $T^*SO(3) \times \mathbb{R}$). If we denote by $\mathfrak{g}^*$ the dual of the Lie algebra of G, then the quotient space $\mathfrak{g}^* \times \mathbb{R}$ inherits a Jacobi structure.
- Moreover, the evolution vector field describes the dynamics of the reduced system, it is possible to derive the corresponding single generation formalism in the same way that we have shown and it is also possible to define the corresponding discretizations.

Thank you for your attention!