Contact geometry for simple thermodynamical systems with friction

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By means of the Jacobi structure associated with a contact structure, we use the so-called evolution vector field to propose a new characterization of isolated thermodynamical systems with friction, a simple but important class of thermodynamical systems which naturally satisfy the first and second laws of thermodynamics, i.e. total energy preservation of isolated systems and non-decreasing total entropy, respectively. We completely clarify its qualitative dynamics, the underlying geometrical structures and we also show how to apply discrete gradient methods to numerically integrate the evolution equations for these systems.

1. Introduction

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 (see [1,2]) 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 [3] 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 (see also [4]). These approaches have proved to be very useful for the description of complex thermodynamical systems and also facilitate their numerical integration. Also, Gay-Balmaz and Yoshimura [5,6] have recently 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 [7–9]. 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 (see §2). 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 [10,11].

Another approach to the dynamics of thermodynamical processes is the one used in [12,13], which is based on homogeneous symplectic Hamiltonian systems. Since the homogeneous symplectic Hamiltonian formulation unifies, e.g. the energy and entropy representation of thermodynamic systems, it is not completely equivalent to the contact Hamiltonian vector field approach (here the contact descriptions of energy and entropy representation are really different, although conformally equivalent). 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 [14–16]. The approach taken in our paper is fundamentally different from the standard contact geometry approach to thermodynamic systems. In the latter, the state space is the so-called thermodynamic phase space of extensive and intensive variables, while in the present paper, when applied to a thermodynamical context, the state space is basically the space of extensive variables (including entropy, but excluding initially energy).

In §§2 and 3, based on the two laws of thermodynamics and on contact geometry, we study the thermodynamical evolution in terms of a different vector field from the contact Hamiltonian vector field, which is called the evolution or horizontal vector field, and then we describe the dynamics associated to this vector field. The evolution vector field is defined in terms of the canonical bi-vector associated with the contact structure. We will check that it satisfies, for Hamiltonian functions, the two laws of thermodynamics. Contrary to the Hamiltonian vector field, the evolution vector field does not preserve the contact structure. However, it preserves the Hamiltonian and it is tangent to constant energy Legendrian submanifolds. Moreover, it coincides with the Hamiltonian vector field on the zero level set of the Hamiltonian. In particular, the evolution vector field would produce the same dynamics for equilibrium states as the Hamiltonian vector field on the formalism of [11]. Moreover, the relation with the single generation formalism is stated without the use of any additional geometric structure to deduce the equations of thermodynamics, thus being a more natural construction. In §4, we analyse the possibility of numerically integrating the thermodynamical equations using discrete gradient methods (see for instance [17–19]), since the evolution vector field is associated with a bi-vector field. Finally, at the end of §4, we develop a discrete Lagrangian formalism adapted to the contact structure and to the evolution vector field. Using this approach, we deduce an integrator capturing the most important features of the dynamics.

2. Contact geometry

In this section, we consider some ingredients of contact geometry that we will need in the sequel [8,9,16].

Let $M$ be a differentiable manifold of dimension $2n + 1$ and a 1-form $\eta$ on $M$. We say that $\eta$ is a contact 1-form if $\eta \wedge (d\eta)^n \neq 0$ at every point. Then, we call $(M, \eta)$ 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

$$\flat : \mathfrak{X}(M) \longrightarrow \Omega^1(M)$$

$$X \mapsto i_X d\eta + \eta(X) \eta$$

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 neighbourhood of every point $x \in M$, such that the contact $1$-form $\eta$ and the Reeb vector field are

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

Define the bi-vector $\Lambda$ on $M$ by

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

In canonical coordinates,

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

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

$$\sharp_A : \Omega^1(M) \to \mathfrak{X}(M),$$

by $\langle \beta, \sharp_A(\alpha) \rangle = \Lambda(\alpha, \beta)$ 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

$$X_f = \sharp_A(df) - fR,$$

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**

$$E_f = \sharp_A(df) = X_f + fR$$

or

$$\flat(E_f) = df - R(f) \eta.$$ 

In canonical coordinates,

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

**Remark 2.1.** In the next section, 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.
The pair \((A, E = -R)\) is a particular case of Jacobi structure since it satisfies
\[
[A, A] = 2E \wedge A \quad \text{and} \quad [A, E] = 0.
\]
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 \(\{,\} : C^\infty(M, \mathbb{R}) \times C^\infty(M, \mathbb{R}) \to C^\infty(M, \mathbb{R})\) 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,
\[
\{f, g\} = \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i} - \frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial S} \left( p_i \frac{\partial g}{\partial p_i} - g \right) + \frac{\partial g}{\partial S} \left( p_i \frac{\partial f}{\partial p_i} - f \right).
\]
It is also interesting for us to introduce the bracket (Cartan bracket) that does not obey the Jacobi identity
\[
\{f, g\} = \Lambda(df, dg)
\]
\[
= \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q^i} - \frac{\partial f}{\partial q^i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial S} \left( p_i \frac{\partial g}{\partial p_i} \right) + \frac{\partial g}{\partial S} \left( p_i \frac{\partial f}{\partial p_i} \right).
\]
The main example of contact manifold along this paper 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 \(\theta_Q\) 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 \(\Lambda_0\) and an extra term that describes the thermodynamical behaviour. That is,
\[
\{f, g\}_\Delta = \{f, g\}_\Lambda - \frac{\partial f}{\partial S} \Delta g + \frac{\partial g}{\partial S} \Delta f,
\]
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 [3] as
\[ [f, g] = \{ f, g \}_\Lambda + \{ f, g \}_\Delta. \] (2.3)

Now, we will discuss some interesting properties of the qualitative behaviour of the evolution vector field \( \mathcal{E}_f \). In [20] appears a similar result for contact Hamiltonian vector fields (see also [8]).

**Proposition 2.2.** The Lie derivative of the contact form \( \eta \) with respect to the evolution vector field \( \mathcal{E}_f \) associated with 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 (see [9]):

\[ \mathcal{L}_{\mathcal{E}_f} \eta = \mathcal{L}_{X_f + R} \eta = \mathcal{L}_{X_f} \eta + \mathcal{L}_{R} \eta \]
\[ = -R(f)\eta + (i_R \eta) df = -R(f)\eta + df. \]

**Theorem 2.3.** Let \( \mathcal{L}_f = f^{-1}(c) \) be a level set of \( f : M \to \mathbb{R} \) where \( c \in \mathbb{R} \). We assume that \( \mathcal{L}_c(f) \neq \emptyset \) 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 \( \Delta_c \) 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 \( \omega_c \) 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 \( \ker \eta = \text{span} \{ R \} \)) is transverse to \( T_p \mathcal{L}_c(f) \). But since \( \eta_p \wedge df|^V \neq 0 \), then \( df|_V \) is non-degenerate for every subspace \( V \) transverse to \( \ker \eta \). Therefore, \( \omega_c \) is also non-degenerated.

For the second part, we first remark that \( \mathcal{E}_f(f) = 0 \), hence \( (i_c)_* \mathcal{E}_f = \mathcal{E}_f \big|_{\mathcal{L}_c(f)} \) is a well-defined vector field. By proposition 2.2 and Cartan’s identity
\[ i_{\mathcal{E}_f} df = -R(f)\eta + df, \]
Pulling back by \( i_c \), we get
\[ i_{(i_c)_* \mathcal{E}_f} df = -(R(f) \circ i_c)i_c^* \eta + df = -(R(f) \circ i_c) i_c^* \eta, \]
dividing by \( -(R(f) \circ i_c) \),
\[ -i_{(i_c)_* \mathcal{E}_f} df = i_{(i_c)_* \mathcal{E}_f} \omega_c = i_c^* \eta. \]
Thus, \( (i_c)_* (\mathcal{E}_f/R(f)) = \Delta_c \), as we wanted to show.

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
\[ dt = \frac{1}{R(f)} \, d\tau. \]
Remark 2.4. 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 $(dt, \omega_Q)$ (see [21]).

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.

3. Simple mechanical systems with friction

In this section, 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

$$L: TQ \times \mathbb{R} \rightarrow \mathbb{R},$$

$$\quad \quad (v_q, S) \mapsto L(v_q, S),$$

where $Q$ is the configuration manifold describing the mechanical part of the thermodynamical system, $TQ$ is the tangent bundle with canonical projection $\tau_Q: TQ \rightarrow Q$ 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 and the mapping $FL: TQ \times \mathbb{R} \rightarrow T^*Q \times \mathbb{R}$ is a local diffeomorphism, where

$$FL(q^i, \dot{q}^i, S) = (q^i, \frac{\partial L}{\partial \dot{q}^i} S)$$

is the Legendre transform. Then, we may define a Hamiltonian function $H: T^*Q \times \mathbb{R} \rightarrow \mathbb{R}$ 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

$$\frac{dq^i}{dt} = \frac{\partial H}{\partial p_i},$$

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q^i} - p_i \frac{\partial H}{\partial S},$$

$$\frac{dS}{dt} = p_i \frac{\partial H}{\partial p_i}.$$

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, i.e. non-decreasing entropy production.
Proposition 3.1. The integral curves of $\mathcal{E}_H$ satisfy the following properties:

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

Proof. Both are a direct consequence of the definition of the evolution vector field $\mathcal{E}_H = \sharp A(dH)$. \[\square\]

Assume that the Hamiltonian $H$ is given by

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

(3.1)

where $(g^{ij})$ is positive semi-definite (for instance, it is associated with 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 3.2. The integral curves of $\mathcal{E}_H$ satisfy the following properties:

1. **First law of thermodynamics**: $$
dH/dt = 0 \quad (\text{preservation of the total energy});$$

2. **Second law of thermodynamics**: $$
dS/dt = \Delta H \geq 0 \quad (\text{total entropy of an isolated system never decreases}).$$

Proof. It is a direct consequence of proposition 3.1 and $\Delta H = p_is^ijp_j \geq 0$. \[\square\]

If we express the dynamics in terms of the brackets defined in (2.3) we have that

$$
\dot{f} = \{f, H\}_T + \{f, H\}_\Delta.
$$

(3.2)

Obviously, $\{H, H\}_T = \{H, H\}_\Delta = 0$ (first law) and $\{S, H\}_T = 0$ and $\{S, H\}_\Delta = \Delta H \geq 0$ (second law). Observe that in equation (3.2) both brackets are using the function $H$ as ‘generator’. This is the reason that typically this formalism is known as single generator formalism [3].

**Example 3.3 (Linearly damped system).** 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 $\mathcal{E}_H = \sharp A(dH)$ 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

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

Obviously $\dot{H} = 0$ and $\dot{S} \geq 0$. 
In the Lagrangian side, we obtain the system given by
\[ m\ddot{q} = -V'(q) - \gamma m\dot{q} \]
and
\[ \dot{S} = m\dot{q}^2. \]
Observe that in this system the friction force is given by the map \( F_{fr}: TQ \to T^*Q \) given by
\[ F_{fr}(q, \dot{q}) = \gamma \dot{q} \dot{q}^* \].

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 \( T = \partial H / \partial S = -\partial L / \partial S = \gamma > 0 \) represents the temperature of the thermal bath. These equations coincide with the set of equations proposed in [5,6] for this particular choice of Lagrangian \( L \) and friction force \( F_{fr} \). Observe that, in this particular example, the temperature \( T = \gamma \) these equations are only defined for values \( \gamma > 0 \).

Observe that the two brackets are
\[ \{f, g\}_0 = \frac{\partial f}{\partial p} \frac{\partial g}{\partial q} - \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} \]
and
\[ \{f, g\}_\Delta = p \frac{\partial g}{\partial S} \frac{\partial f}{\partial p} - p \frac{\partial f}{\partial S} \frac{\partial g}{\partial p} \]
In particular,
\[ \{H, g\}_0 = \frac{p}{m} \frac{\partial g}{\partial q} \frac{\partial}{\partial q} V'(q) \]
\[ \{H, g\}_\Delta = \frac{p^2}{m} \frac{\partial g}{\partial S} - \gamma p \frac{\partial g}{\partial p} \]
and
\[ \mathcal{E}_H(g) = \dot{g} = \{H, g\}_0 + \{H, g\}_\Delta. \]
Therefore, it is clear that \( \{H, H\}_0 = 0 \) and \( \{H, H\}_\Delta = 0 \) (by skew-symmetry) and \( \{H, S\}_0 = 0 \) and \( \{H, S\}_\Delta = p^2 / m \geq 0 \).

4. Geometric integration of simple thermodynamical systems

(a) Integration based on discrete gradients

Numerical methods for general thermodynamical systems are implemented usually using the metriplectic formalism (see [22,23]), however in our case, for the examples that we are considering, we can easily adapt the construction of discrete gradient methods to the bivector \( \Lambda \).

For simplicity, we will assume that \( Q = \mathbb{R}^n \). Then the systems that we want to study are described by the ODEs
\[ \dot{x} = (\sharp_\Lambda)(\nabla H(x)), \]
with \( x = (q^i, p^i, S) \in T^*Q \times \mathbb{R} \), the map \( H: T^*Q \times \mathbb{R} \to \mathbb{R} \) is the Hamiltonian function and \( \nabla H(x) \in \mathfrak{X}(T^*Q \times \mathbb{R}) \) is the standard gradient in \( T^*Q \times \mathbb{R} \) identified with \( \mathbb{R}^{2n+1} \), with respect to the euclidean metric.

Using discretizations of the gradient \( \nabla H(x) \), it is possible to define a class of integrators which preserve the first integral \( H \) exactly.
Definition 4.1. Let \( H : \mathbb{R}^N \to \mathbb{R} \) be a differentiable function. Then \( \tilde{\nabla} H : \mathbb{R}^{2N} \to \mathbb{R}^N \) is a discrete gradient of \( H \) if it is continuous and satisfies
\[
\tilde{\nabla} H(x, x')^T (x' - x) = H(x') - H(x), \quad \text{for all } x, x' \in \mathbb{R}^N, \tag{4.1a}
\]
\[
\tilde{\nabla} H(x, x) = \nabla H(x), \quad \text{for all } x \in \mathbb{R}^N. \tag{4.1b}
\]

Some examples of discrete gradients are (see [24] and references therein)

— The **mean value (or averaged) discrete gradient** given by
\[
\tilde{\nabla}_1 H(x, x') := \int_0^1 \nabla H((1 - \xi)x + \xi x') \, d\xi, \quad \text{for } x' \neq x. \tag{4.2}
\]

— The **midpoint (or Gonzalez) discrete gradient** given by
\[
\tilde{\nabla}_2 H(x, x') := \nabla H \left( \frac{1}{2} (x' + x) \right) + \frac{H(x') - H(x) - \nabla H \left( \frac{1}{2} (x' + x) \right)^T (x' - x)}{|x' - x|^2} (x' - x), \tag{4.3}
\]
for \( x' \neq x \).

— The **coordinate increment discrete gradient** where each component given by
\[
\tilde{\nabla}_3 H(x, x')_i = \frac{H(x'_1, \ldots, x'_i, x_{i+1}, \ldots, x_n) - H(x'_1, \ldots, x'_{i-1}, x_i, \ldots, x_n)}{x'_i - x_i}, \quad 1 \leq i \leq N, \text{ when } x'_i \neq x_i, \text{ and}
\]
otherwise.

Let \( H : T^*Q \times \mathbb{R} \to \mathbb{R} \) be the Hamiltonian function. Once a discrete gradient \( \tilde{\nabla} H \) has been chosen, it is straightforward to define an energy-preserving integrator by, for instance, using the midpoint discrete gradient
\[
\frac{x_{k+1} - x_k}{h} = (\tilde{\gamma}(A))(x_k + x_{k+1})/2 \tilde{\nabla}_2 H(x_k, x_{k+1}), \tag{4.4}
\]
where \( A \) is the bivector associated with the canonical contact structure \( \eta_Q \) of \( T^*Q \times \mathbb{R} = \mathbb{R}^{2n+1} \), given in local coordinates by (2.2).

As in the continuous case, it is immediate to check that \( H \) is exactly preserved using (4.4) and the skew-symmetry of \( A \)
\[
H(x_{k+1}) - H(x_k) = \tilde{\nabla}_2 H(x_k, x'_{k+1})^T (x_{k+1} - x_k) = hA(\tilde{\nabla}_2 H(x_k, x_{k+1}), \tilde{\nabla}_2 H(x_k, x_{k+1})) = 0.
\]

On the other hand, by (4.4), the entropy satisfies
\[
S_{k+1} - S_k = hA(\tilde{\nabla}_2 H(x_k, x_{k+1}), dS).
\]
If \( H \) is of the form (3.1) with \( V \) a quadratic function then
\[
H(x_{k+1}) - H(x_k) = dH \left( \frac{x_k + x_{k+1}}{2} \right) (x_{k+1} - x_k).
\]
In fact, this is a well-known property of quadratic functions. Hence, we must have
\[
dH \left( \frac{x_k + x_{k+1}}{2} \right) = \tilde{\nabla}_2 H(x_k, x_{k+1}).\]
so that
\[ S_{k+1} - S_k = h \Lambda \left( dH \left( \frac{x_k + x_{k+1}}{2} \right), dS \right) = h \left( \frac{p_k^i + p_{k+1}^i}{2} \right) \frac{\partial H}{\partial p^i} \left( \frac{x_k + x_{k+1}}{2} \right) \geq 0, \]
since by (2.2), we have that
\[ \Lambda (dq^i, dS) = 0, \quad \Lambda (dp^i, dS) = p_i \quad \text{and} \quad \Lambda (dS, dS) = 0. \]

**Example 4.2.** Consider the Hamiltonian function \( H: T^* Q \to \mathbb{R} \) given by
\[ H(q, p, S) = \frac{p^2}{2} + \frac{q^2}{2} + \gamma S, \quad (4.5) \]
where \( Q = \mathbb{R} \), which is the Hamiltonian function associated with the damped harmonic oscillator.

Now, if we may apply the midpoint discrete gradient and the associated integrator given by (4.4), we obtain the following integrator:
\[
q_1 = \frac{2\gamma h q_0 - h^2 q_0 + 4h p_0 + 4q_0}{2\gamma h + h^2 + 4}, \\
p_1 = -\frac{2\gamma h p_0 + h^2 p_0 + 4h q_0 - 4p_0}{2\gamma h + h^2 + 4}, \\
S_1 = \frac{S_0 h^4 + (4S_0 \gamma + 4q_0^2) h^3 + (4S_0 \gamma^2 - 16p_0 q_0 + 8S_0) h^2}{(2\gamma h + h^2 + 4)^2} + \frac{(16S_0 \gamma + 16p_0^2) h + 16S_0}{(2\gamma h + h^2 + 4)^2}. \quad (4.6)
\]

Of course, using equations (4.6), we obtain an integrator with constant energy and increasing entropy. In figure 1, we can see that the qualitative behaviour of the integrator is fairly accurate, while in figure 2 we see the entropy increases at the same rate as the exact one.

**b) Integration based on discrete Herglotz principle**

**(i) The geometric setting**

Let \( L: TQ \times \mathbb{R} \to \mathbb{R} \) be a regular Lagrangian function as in §3 (see [25,26]). As before, let us 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 \( \mathbb{R} \).

Given a Lagrangian function \( L \), using the canonical endomorphism \( S \) on \( TQ \) locally defined by
\[ S = dq^i \otimes \frac{\partial}{\partial q^i}, \]
one can construct a 1-form \( \lambda_L \) on \( TQ \times \mathbb{R} \) given by
\[ \lambda_L = S^*(dL), \]
where now \( S \) and \( S^* \) are the natural extensions of \( S \) and its adjoint operator \( S^* \) to \( TQ \times \mathbb{R} \) [27].

Therefore, we have that
\[ \lambda_L = \frac{\partial L}{\partial q^i} dq^i. \]

Now, the 1-form on \( TQ \times \mathbb{R} \) given by \( \eta_L = dS - \lambda_L \), or, in local coordinates, by
\[ \eta_L = dS - \frac{\partial L}{\partial q^i} dq^i, \]
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

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

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 $\Delta = \dot{q}^j (\partial / \partial \dot{q}^j)$ is the natural extension of the Liouville vector field on $\mathcal{Q} \times \mathbb{R}$. Therefore, in local coordinates, we have that

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

Denote by $b_L : T(\mathcal{Q} \times \mathbb{R}) \to T^*(\mathcal{Q} \times \mathbb{R})$ the vector bundle isomorphism given by

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

where $\eta_L$ is the contact form on $\mathcal{Q} \times \mathbb{R}$ previously defined. We shall denote its inverse isomorphism by $\sharp_L = (b_L)^{-1}$.

Let $\xi_L$ be the unique vector field satisfying the equation

$$b_L(\xi_L) = dE_L - (R_L E_L + E_L) \eta_L. \quad (4.7)$$

A direct computation from equation (4.7) shows that if $(q^i(t), \dot{q}^i(t), S(t))$ is an integral curve of $\xi_L$, then it satisfies the generalized Euler–Lagrange equations considered by G. Herglotz in 1930:

$$\begin{align*}
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} &= \frac{\partial L}{\partial \dot{q}^i} \frac{\partial S}{\partial \dot{q}^i}, \\
\dot{S} &= L(q^i, \dot{q}^i, S).
\end{align*} \quad (4.8)$$

Now, given a regular Lagrangian function $L$, we may define the bi-vector $\Lambda_L$ on $\mathcal{Q} \times \mathbb{R}$ as in (2.1) associated with the contact form $\eta_L$. Thus,

$$\Lambda_L(\alpha, \beta) = -d\eta_L(\gamma^{-1}_L(\alpha), \gamma^{-1}_L(\beta)), \quad \alpha, \beta \in \Omega^1(\mathcal{Q} \times \mathbb{R}).$$

If $(q^i(t), \dot{q}^i(t), S(t))$ is an integral curve of the evolution vector field $\xi_L$ associated with the contact form $\eta_L$ defined by

$$\xi_L = \sharp_L(dE_L) \text{ or } b_L(\xi_L) = dE_L - (R_L E_L) \eta_L,$$

then it satisfies the thermodynamical Herglotz equations

$$\begin{align*}
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \right) - \frac{\partial L}{\partial q^i} &= \frac{\partial L}{\partial \dot{q}^i} \frac{\partial S}{\partial \dot{q}^i}, \\
\dot{S} &= \dot{q}^i \frac{\partial L}{\partial \dot{q}^i}.
\end{align*} \quad (4.10)$$

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

(ii) Discrete Herglotz equations

Now, we propose to construct a numerical integrator for $\xi_L$ based on a similar method to the discrete Herglotz principle [28,29].

Let $L_d : \mathcal{Q} \times \mathcal{Q} \times \mathbb{R} \to \mathbb{R}$ be a discrete Lagrangian function. Then a possible integrator for the evolution dynamics is

$$D_1 L_d(q_1, q_2, S_1) + (1 + D_3 L_d(q_1, q_2, S_1))D_2 L_d(q_0, q_1, S_0) = 0, \quad (4.11)$$

and the entropy is subjected to

$$S_1 - S_0 = (q_1 - q_0)D_2 L_d(q_0, q_1, S_0). \quad (4.12)$$
Figure 3. Trajectory of (4.13): 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 \( \mathcal{E}_t \). (Online version in colour.)

Figure 4. Hamiltonian of (4.13): using the same initial data and settings from figure 3, we plot the Hamiltonian function along the iterations of the integrator. (Online version in colour.)

**Example 4.3.** Consider again the Hamiltonian function (4.5) of the damped harmonic oscillator. Since \( H \) is regular, we might 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

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

The discrete Herglotz equations (4.11) together with (4.12) give the explicit integrator

\[
\begin{align*}
q_2 &= \frac{\gamma h^2 q_0 + \gamma h^3 q_1 + 4\gamma h q_0 - 4\gamma h q_1 - h^2 q_0 - 2h^2 q_1 - 4q_0 + 8q_1}{h^2 + 4} \\
S_1 &= S_0 + \frac{(q_1 - q_0)^2}{h} - \frac{h}{4} q_1^2 - \frac{q_0^2}{4}.
\end{align*}
\] (4.13)
In figure 3, we plot the integrator given by equations (4.13). 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.

As a last comment, the entropy for equations (4.13) is increasing and the Hamiltonian oscillates before stabilizing around a constant value (cf. figure 4).

5. Conclusion 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 of [3] 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 with a given Lagrangian function $L: TQ \times \mathbb{R} \rightarrow \mathbb{R}$. This would allow us to develop higher order methods in a simple way as in [30]. In recent papers such as [28,29], 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 as in [31] or working with other types of Jacobi manifolds.

For instance, in our paper, we have initially started with contact structures but the proposed framework is also valid for general Jacobi manifolds which naturally covers other interesting examples of thermodynamical systems. As an example, consider a Poisson manifold $(M, \Lambda)$, that is, a differentiable manifold $M$ equipped with a bivector field $\Lambda$ with associated bracket $\{,\}$ verifying that $[\Lambda, \Lambda] = 0$. Let $k \in C^\infty(M)$ and consider the corresponding Hamiltonian vector field for 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 $(\Lambda_k, X_k)$ is a Jacobi manifold [32]. In other words,

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

This structure appears, for instance, in models with heat exchange between different subsystems. As a simple example, consider two simple thermodynamic subsystems (for instance, two ideal gases) [33], which may interact through a conducting wall. The variables are now $(S_1, S_2)$, the entropies of subsystem 1 and 2, respectively. Given a Hamiltonian $H(S_1, S_2) = U(S_1) + U(S_2)$ representing the internal energy composed of the addition of the internal energies of both subsystems, consider now the function

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

where $\lambda > 0$ is the Fourier heat conduction coefficient and $T_i = \partial U/\partial S_i > 0$, $i = 1, 2$, represent the temperatures of both subsystems, respectively. Taking the canonical Poisson structure on $\mathbb{R}^2$

$$A = \frac{\partial}{\partial S_1} \wedge \frac{\partial}{\partial S_2},$$
consider the associated Jacobi manifold \((\Lambda_k, X_k)\) and the corresponding evolution vector field \(\mathcal{E}_H\)

\[
\mathcal{E}_H = \sharp_{\Lambda_k}(dH) = \lambda \left( \frac{\partial U/\partial S_2}{\partial U/\partial S_1} - 1 \right) \frac{\partial}{\partial S_1} - \lambda \left( 1 - \frac{\partial U/\partial S_1}{\partial U/\partial S_2} \right) \frac{\partial}{\partial S_2}
\]

\[
= \lambda \left( \frac{T_2}{T_1} - 1 \right) \frac{\partial}{\partial S_1} + \lambda \left( \frac{T_1}{T_2} - 1 \right) \frac{\partial}{\partial S_2}.
\]

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

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

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 of 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 \(g^*\) the dual of the Lie algebra of \(G\) then the quotient space \(g^* \times \mathbb{R}\) inherits a Jacobi structure. Moreover, the evolution vector field describes the dynamics of the reduced system and it is possible to derive the corresponding single generation formalism for this case in a similar way that the exposed in our paper and moreover to derive the corresponding discretizations (see [34] and references therein).

Data accessibility. https://arxiv.org/abs/2004.01989.

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