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IFAC-PapersOnLine 49-24 (2016) 040–045

About the lift of irreversible thermodynamic systems to the Thermodynamic Phase Space

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Abstract: n this paper, we analyze the different lift of the dynamics of irreversible thermodynamic systems from the Legendre submanifold associated with the thermodynamic properties of the physical system to the full Thermodynamic Phase Space. Firstly, we define a set of Hamiltonian functions which generate a class of equivalent lifts, that it contact vector fields which are equal on some distinguished Legendre submanifold. Secondly we show that how one may construct an equivalent contact vector field which renders attractive of the inverse image of zero by the Hamiltonian function.

Keywords: Nonlinear systems, Stability, Dynamical models, Thermodynamic models, Hamiltonian systems

1. INTRODUCTION

In recent years, the dynamics of open irreversible Thermodynamic systems has been expressed in terms of control systems where the drift and input vector fields are Hamiltonian systems defined on contact manifolds [1]. The contact manifolds correspond to the Thermodynamic Phase Space which is naturally endowed with a contact form associated with Gibbs' form [2]. Contact systems have been defined for reversible transformations Mrugała [2000] and for open systems undergoing irreversible transformations, different definition of control contact systems have been suggested Bravetti et al. [2015], Eberard et al. [2007], Favache et al. [2010, 2009], Grmela [2002], Merker and Krüger [2013], Ramirez et al. [2013b,a].

The practical construction of the contact systems associated with physical systems is however still a matter of debate. Indeed dynamic models of open irreversible thermodynamic systems may in general be expressed in terms of n balance equations of the n independent extensive variables (or any equivalent set of independent dynamic equations in terms of some mixed set of the extensive and intensive variables). It is very current to express the dynamical behaviour of the system in terms of $(2n+1)$ dynamic equations of all extensive and intensive variables of the thermodynamic system. This corresponds to lift the n independent balance equations to the complete Thermodynamic Phase Space. This lift may be performed in various ways Eberard et al. [2007], Favache et al. [2009], Gromov and Caines [2015], Ramirez et al. [2013b] which lead to conservative contact vector fields which are equal on the Legendre submanifold (we call them then *equivalent*) but might have very different properties on the complete Thermodynamic Phase Space. In this paper we shall discuss a class of equivalent contact vector field with respect to some stability properties.

In the section 2 we shall briefly recall the main definitions of conservative contact vector fields arising from the lift of an nonlinear control system and conclude with precise motivations of the paper. In the section 3 we shall define a class of equivalent conservative contact vector fields and analyze the attractivity of some submanifolds including the Legendre submanifold.

2. BRIEF REMINDER AND MOTIVATION

2.1 Equilibrium models and dynamical models

Equilibrium model A physical system is first defined by its thermodynamic properties, also called equilibrium model. They are defined on the Thermodynamic Phase Space, denoted by $\mathcal{M}$, which is composed of the set of $n+1$ *extensive variables*, denoted by $x = \left(x^i\right)_{i=0,\ldots,n}$, (such as internal energy, volume, number of moles of chemical species, entropy) and the n conjugated *intensive variables*, denoted by $p = (p_i)_{i=1,\ldots,n}$, (such as pressure, chemical potential and temperature). The thermodynamic properties are then defined by a differential relation, called *Gibbs' relation* on the extensive and intensive variables. Actually these relations have been interpreted geometrically by Gibbs Gibbs [1873] and later have let to endow the Thermodynamic Phase Space with a *contact form,* denoted by θ in the sequelArnold [1989], Mrugała [2000] [3].

[1] We shall call these systems, *contact systems* in the sequel.

[2] The contact manifold defined by the contact form is the equivalent of the *symplectic manifold* associated with the configuration-momentum space of mechanical systems Herman [1973], Arnold [1989].

[3] The reader is referred to the classical textbooks [Libermann and Marle 1987, chap. V.] and [Arnold 1989, app. 4.] for detailed

Peer review under responsibility of International Federation of Automatic Control.
10.1016/j.ifacol.2016.10.751

In a set of canonical coordinates this contact form is expressed as

$$\theta = dx_0 - \sum_{i=1}^{n} p_i dx_i \tag{1}$$

The Thermodynamic properties of a system define the physical admissible state space (where Gibbs relation is satisfied) and it may be shown that the latter may be defined in terms of a Legendre submanifold $\mathcal{L} \subset \mathcal{M}$ of the Thermodynamic Phase Space [4] . In practice the thermodynamic properties of thermodynamic systems are given in terms of some generating functions, called *thermodynamic potentials*, such as the internal energy, the enthalpy or the free energy (seeEberard et al. [2007], Favache et al. [2010], Mrugała [2000] for detailed examples). One canonical choice is to choose the extensive variables as coordinates of the Legendre submanifold and the internal energy (or total energy for multiphysical systems), as its generating function $U \in C^{\infty}(\mathbb{R}^n)$ as follows

$$\mathcal{L}_U = \left\{ x_0 = U(x), x = x, p = \frac{\partial U}{\partial x}(x),\ x \in \mathbb{R}^n \right\} \tag{2}$$

Dynamical model For the simplicity, let us express the system's properties using n extensive variables $x = \left(x^i\right)_{i=1,..,n} \in \mathbb{R}^n$ as independent coordinates and use the internal energy to define the equilibrium properties (i.e. the Legendre submanifold $\mathcal{L}$). And let us assume that the system of balance equations may be written as the nonlinear control system

$$\frac{dx}{dt} = f\left(x, \frac{\partial U}{\partial x}\right) + \sum_{j=1}^{p} g^j \left(x, \frac{\partial U}{\partial x}\right) u_j \tag{3}$$

where the drift vector field f and the control vector fields g^j depend explicitly on the independent set of extensive variables x and their conjugated intensive variables $\frac{\partial U}{\partial x}$.

2.2 Lift of the balance equations to the Thermodynamic Phase Space

As written in the introduction, it is the use in Thermodynamics and Chemical Engineering to express the balance equations in actually all the extensive and intensive variables, that means on the whole Thermodynamic Phase Space. However there are infinitely many ways to perform the lift of the balance equations (3) to the Thermodynamic Phase Space.

For instance in Gromov and Caines [2015], this lift is expressed in canonical coordinates as follows. Consider a Legendre submanifold $\mathcal{L}_U$ generated by the internal energy $U(x)$, defined in a set of canonical coordinates according to (2) and a smooth vector field $f(x)$ with components $f_i(x)$ defined on it. The lift to the Thermodynamic Phase Space is defined by the vector field, in canonical coordinates

$$\begin{aligned} \tilde{X} =& \left(\sum_{i=1}^{n} p_i f_i(x)\right) \frac{\partial}{\partial x^0} + \sum_{i=1}^{n} f_i(x) \frac{\partial}{\partial x^i} \\ &+ \sum_{j=1}^{n} \left(\sum_{i=1}^{n} f_i(x) \frac{\partial^2 U}{\partial x^i \partial x^j}\right) \frac{\partial}{\partial p_j} \end{aligned} \tag{4}$$

which is tangent to the Legendre submanifold $\mathcal{L}_U$ [Gromov and Caines 2015, Th. 1].

In this paper we would like to follow the route opened in Mrugała [2000] and Grmela and Öttinger [1997] and lift the balance equations to a contact vector field which preserves the contact distribution associated with the contact form (Gibbs' form) on the Thermodynamic Phase Space.

Definition 1. A (smooth) vector field X on the contact manifold $\mathcal{M}$ is a *contact vector field* with respect to a contact form θ if and only if there exists a smooth function $\rho \in C^{\infty}(\mathcal{M})$ such that

$$L_X \theta = \rho\theta, \tag{5}$$

where $L_X\cdot$ denotes the Lie derivative with respect to the vector field X. It is called a *strict contact vector field* if $\rho = 0$ [5].

It appears then that the lift (4) , is not a contact vector field.

Lemma 2. The vector field (4) is a contact vector field if and only if the vector field $f = 0$.

Proof. Indeed with $\theta = dx^0 - p_i dx^i$ and $d\theta = -dp_i \wedge dx^i$, one obtains

$$\begin{aligned} L_{\tilde{X}}\theta &= di_{\tilde{X}}\theta + i_{\tilde{X}} d\theta \\ &= d\left(p^T f(x) - p^T f(x)\right) + i_{\tilde{X}} d\theta \\ &= \sum_{i=1}^{n} f_i(x)\, dp_i - \sum_{i,j=1}^{n} \frac{\partial^2 U}{\partial x^i \partial x^j} f_j(x)\, dx^i \end{aligned}$$

Considering the expression of the contact form (1) it follows the vector field satisfies $L_{\tilde{X}}\theta = \rho\,\theta$ iff $\rho = 0$ and $f = 0$.

Actually one may lift the system of balance equations (3) to the complete Thermodynamic Phase Space by defining the following contact Hamiltonian functions

$$K_0 = \left(\frac{\partial U}{\partial x} - p\right)^{\top} f(x, \frac{\partial U}{\partial x}); \quad K_c^j = \left(\frac{\partial U}{\partial x} - p\right)^{\top} g^j(x, \frac{\partial U}{\partial x}) \tag{8}$$

By construction, the contact vector field X_K, generated by the function $K = K_0 + \sum_{j=1}^{p} K_c^j$, leaves invariant the the Legendre submanifold $\mathcal{L}_U$ generated by the internal energy $U(x)$ and its restriction to $\mathcal{L}_U$ coincides with (3).

presentations and to Eberard et al. [2007] for a presentation in the context of systems' theory.

[4] A Legendre submanifold is an integral manifold of θ, of maximal dimension.

[5] There exists a unique real function K , called generating function, associated with a contact vector field X is

$$K = i_X \theta \tag{6}$$

and called here *contact Hamiltonian.* The contact vector field generated by the function K is denoted by X_K. The function ρ in (5) is given by

$$\rho = i_E dK \tag{7}$$

where E is the *Reeb vector field* associated with the contact form θ and uniquely defined by $i_E\theta = 1$ and $i_E d\theta = 0$ where i_E denotes the contraction by the vector field E of differential forms.