



### University of Groningen

### Port contact systems for irreversible thermodynamical systems

Eberard, D.; Maschke, B.M.; Schaft, A.J. van der

Published in:

Proceedings of the 44th IEEE Conference on Decision and Control, and the European Control Conference

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version Publisher's PDF, also known as Version of record

Publication date:

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):

Eberard, D., Maschke, B. M., & Schaft, A. J. V. D. (2005). Port contact systems for irreversible thermodynamical systems. In Proceedings of the 44th IEEE Conference on Decision and Control, and the European Control Conference (pp. 5977-5982). University of Groningen, Johann Bernoulli Institute for Mathematics and Computer Science.

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: https://www.rug.nl/library/open-access/self-archiving-pure/taverneamendment.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): http://www.rug.nl/research/portal. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Download date: 04-06-2022

## Port contact systems for irreversible thermodynamical systems

D. Eberard, B.M. Maschke and A.J. van der Schaft

Abstract—In this paper we propose a definition of control contact systems, generalizing input-output Hamiltonian systems, to cope with models arising from irreversible Thermodynamics. We exhibit a particular subclass of these systems, called conservative, that leaves invariant some Legendre submanifold (the geometric structures associated with thermodynamic properties). These systems, both energy-preserving and irreversible, are then used to analyze the loss-lessness of these systems with respect to different generating functions.

Index Terms—Port Hamiltonian systems, Irreversible Thermodynamics, contact vector fields, lossless systems

#### I. Introduction

The objective of this paper is to elaborate on the definition of conservative systems defined on contact manifolds given in [4] and to analyze their properties with respect to losslessness. In [4], we have proposed a generalization of port Hamiltonian systems which allows to cope with models arising from Irreversible Thermodynamics. These systems have been derived from the lift of port Hamiltonian systems [9], [19], [17] on a Thermodynamic Phase Space associated with its state space. These conservative systems on contact manifolds also complete the differential-geometric definition of Reversible Thermodynamics [3], [7], [10], [14], which uses the notion of contact structures [8]. Indeed firstly they use generating function which corresponds to some law of generation of fluxes from non-equilibrium conditions (as thermal non-equilibrium for heat flux etc..). Secondly they complete the system with input and output variables and some input term representing the interaction of the system with its environment. The qualifier conservative is understood that these system conserve the Thermodynamic properties of the system. In this paper we shall firstly propose an alternative definition of the conservative systems defined on contact manifolds defined in [4]. Secondly we shall investigate the losslessness properties of these systems. The sketch of the paper is the following. In section 2 we briefly recall the basic concepts of contact geometry [8] and [2] in the context of Reversible Thermodynamics [7], [10], [14]. In the section 3, we define control contact systems on

D.Eberard and B.M.Maschke are with Laboratoire d'Automatique et de Génie des Procédés UMR CNRS 5007, Université Claude Bernard, Lyon, France eberard@lagep.univ-lyon1.fr and maschke@lagep.univ-lyon1.fr

A.J. van der Schaft is with the Faculty of Mathematical Sciences, University of Twente, Enschede, The Netherlands a.j.vanderschaft@math.utwente.nl

contact manifolds, which may be seen as the analogue of input-output Hamiltonian systems defined on symplectic manifolds [15], [16]. We then give the definition of a subclass of these systems, called conservative, which leave invariant some Legendre submanifold (corresponding to the invariance of some thermodynamical properties) and correspond to an alternative definition of conservative systems on contact manifolds [4]. In the section 4 we analyze the losslessness properties of this systems with respect to different functions.

# II. CONTACT STRUCTURES FOR REVERSIBLE THERMODYNAMICS

In this section we shall briefly recall the basic concepts of contact geometry (following [8] and [2]) in the context of Reversible Thermodynamics (see [14] and the references herein). First we recall the canonical state space, called Thermodynamic Phase Space, in which the thermodynamic properties of a system are defined. It has a canonical structure, called contact structure, which is related to the Gibb's form and plays an analogous role as the symplectic structure for Lagrangian or Hamiltonian systems.

Let  $\mathcal{M}$  be an 2n+1-dimensional, connected, differentiable manifold of class  $C^{\infty}$ .

Definition 1 ([8]): A Pfaffian equation on  $\mathcal{M}$  is a vector subbundle  $\mathcal{E}$  of rank 1 of  $T^*\mathcal{M}$ . The pair  $(\mathcal{M}, \mathcal{E})$  is a strictly contact structure if there exists a form  $\theta$  of constant class 2n+1, called contact form, that determines  $\mathcal{E}$ .

Using Darboux's theorem, one shows the existence of canonical coordinates  $(x^0, x^1, \dots, x^n, p_1, \dots, p_n)$  in a neighborhood V of any  $x \in \mathcal{M}$  such that

$$\theta_{|V} = \mathrm{d}x^0 - p_i \mathrm{d}x^i. \tag{1}$$

Such structures appears in the differential-geometric representation of thermodynamic systems [7], [10].

Example 1: According to [7], one may define the thermodynamic phase space  $\mathcal{T}$ , associated with some thermodynamic system, as

$$\mathcal{T} := \mathbb{R} \times T^* \mathcal{N},\tag{2}$$

where  $\mathcal{N}$  is the *n*-dimensional manifolds of extensives variables x. With the canonical coordinates given above,  $x^0$  denotes the energy U and the pairs  $(x^i, p_i)$  denote the pairs of conjugated extensives (as the entropy S, the pressure P or the number of mole N) and intensives (as the temperature T, the volume V and the chemical potential  $\mu$ ) variables. In this case, the contact form is

then closely related to Gibb's relation obtained where the contact form vanishes :

$$dU - TdS + PdV - \mu_i dN_i = 0. (3)$$

Actually Gibb's relation corresponds to the definition of a canonical submanifold of a contact structure, called Legendre submanifold and playing an analogous role as Lagrangian submanifolds for symplectic structures.

Definition 2 ([8]): A Legendre submanifold of a (2n + 1)-dimensional contact manifold  $(\mathcal{M}, \mathcal{E})$  is an n-dimensional submanifold  $\mathcal{L}$  of  $\mathcal{M}$  that is an integral manifold of  $\mathcal{E}$ .

Legendre submanifolds are locally generated by some generating function.

Theorem 1 ([1]): For a given set of canonical coordinates and any partition  $I \cup J$  of the set of indices  $\{1, \ldots, n\}$  and for any differentiable function  $F(x^I, p_J)$  of n variables,  $i \in I, j \in J$ , the formulas

$$x^{0} = F - p_{J} \frac{\partial F}{\partial p_{J}}, \quad x^{J} = -\frac{\partial F}{\partial p_{J}}, \quad p_{I} = \frac{\partial F}{\partial x^{I}}$$
 (4)

define a Legendre submanifold of  $\mathbb{R}^{2n+1}$  denoted  $\mathcal{L}_F$ . Conversely, every Legendre submanifold of  $\mathbb{R}^{2n+1}$  is defined in a neighborhood of every point by these formulas, for at least one of the  $2^n$  possible choices of the subset I.

Example 2: For thermodynamic systems, the generating functions are potentials such as the internal energy, the free energy etc. And the associated Legendre submanifold defines the Thermodynamic properties of some system. For instance, consider a Legendre submanifold generated by the Gibbs free energy G of an ideal gas

$$G(T, P, N) = 5/2R(1-ln(T/T_0))-NT(s_0-Rln(P/P_0))$$
,

where R is the ideal gas constant and  $P_0, T_0, s_0$  are some chosen references. The Legendre submanifold then obtained is

$$\begin{cases} x^{0} = 3/2NRT = U \\ x^{1} = Ns_{0} + 5/2NRln(T/T_{0}) - RNln(P/P_{0}) = S \\ x^{2} = NRT/P = V \\ p_{3} = 5/2RT - TS/N = \mu \end{cases}$$

Notice that the coordinate  $x^0$  corresponds to the internal energy U and that the third equation correspond to the property of an ideal gas (the state equation of an ideal gas).

Finally we shall recall the definition of the class of vector fields, called contact vector fields, which preserve the contact structure and may be characterized using the following result.

Proposition 1 ([8]): A vector field X on  $(\mathcal{M}, \mathcal{E})$  is an contact vector field if and only if there exists a differentiable function  $\rho$  such that

$$\mathcal{L}(X)\,\theta = \rho\,\theta,\tag{5}$$

where  $\mathcal{L}(X)$  denotes the Lie derivative with respect to the vector field X. When  $\rho$  vanishes, X is an infinitesimal automorphism of the contact structure.

It is worth noting that the set of contact vector fields forms a Lie subalgebra of the Lie algebra of vector fields on  $\mathcal{M}$ .

Analogously to the case of Hamiltonian vector fields, one may associate some generating function to the contact vector fields. Actually there exists an isomorphism  $\Phi$  between contact vector fields and differentiable function on  $\mathcal{M}$  which associate to a contact vector field X a function called *contact Hamiltonian* and defined by :

$$\Phi(X) = i(X)\theta, \tag{6}$$

where i(X) denotes the contraction of a form by the vector field X. In the sequel we shall denote the contact vector field associated with a function f by :

$$X_f = \Phi^{-1}(f). \tag{7}$$

The contact vector field  $X_f$  may be expressed in canonical coordinates in terms of the generating function, as follows:

$$X_{f} = \left( f - \sum_{k=1}^{n} p_{k} \frac{\partial f}{\partial p_{k}} \right) \frac{\partial}{\partial x^{0}} + \frac{\partial f}{\partial x^{0}} \left( \sum_{k=1}^{n} p_{k} \frac{\partial}{\partial p_{k}} \right) + \sum_{k=1}^{n} \left( \frac{\partial f}{\partial x^{k}} \frac{\partial}{\partial p_{k}} - \frac{\partial f}{\partial p_{k}} \frac{\partial}{\partial x^{k}} \right).$$
(8)

Furthermore the isomorphism  $\Phi$  transports the Lie algebra structure on the differentiable function on  $\mathcal{M}$  and defines the following bracket that we shall use in the sequel:

$$\{f,g\} = i([X_f, X_g])\theta, \tag{9}$$

whose expression in canonical coordinates is given by

$$\{f,g\} = \sum_{k=1}^{n} \left( \frac{\partial f}{\partial x^{k}} \frac{\partial g}{\partial p_{k}} - \frac{\partial g}{\partial x^{k}} \frac{\partial f}{\partial p_{k}} \right) + \left( f - \sum_{k=1}^{n} p_{k} \frac{\partial f}{\partial p_{k}} \right) \frac{\partial g}{\partial x^{0}} - \left( g - \sum_{k=1}^{n} p_{k} \frac{\partial g}{\partial p_{k}} \right) \frac{\partial f}{\partial x^{0}}.$$

$$(10)$$

Example 3: In the context of Thermodynamics, Mrugala [11] has shown that one may define the reversible transformations of thermodynamical systems. For instance, consider a thermodynamic system defined by the submanifold  $\mathcal{L}_U$  generated, in canonical coordinates, by a function  $U(x^i, p_j)$ ,  $i \in I$ ,  $j \in J$ ,  $I \cup J = \{1, ..., n\}$ . The contact vector field with contact Hamiltonian f, given by

$$f = x^0 - U + p_i \frac{\partial U}{\partial p_i},\tag{11}$$

generates a reversible transformation of the thermodynamic system. An important property of the reversible transformations is that they leave invariant the Legendre submanifold associated with its thermodynamical properties. This may be checked by using the following result [14].

Theorem 2: Let  $(\mathcal{M}, \mathcal{E})$  be a strictly contact manifold and denote  $\theta$  its contact form. Let  $\mathcal{L}$  denote a Legendre

submanifold. Then  $X_f$  is tangent to  $\mathcal{L}$  if and only if f is identically zero on  $\mathcal{L}$ .

Example 4: We recall here the linearized case of the Onsager-Casimir relations presented in [6]. The time evolution of x, in a neighborhood V of an equilibrium state, is governed by

$$\dot{x} = (TJ - D)y \,, \tag{12}$$

where T is the temperature, J a skewsymmetric matrix, D a positive definite matrix and where y coincides with the partial derivative of a potential function  $\phi$  with respect to x on V. In the contact geometry formalism, the author introduces a dissipative potential  $\Theta$ , satisfying some properties (see [6] for details), to define the following contact hamiltonian

$$K = \left(\Theta\left(\frac{\partial\phi}{\partial x}\right) - \Theta(y)\right) + T\left\langle y, J(x)\frac{\partial\phi}{\partial x}\right\rangle , \quad (13)$$

where J(x) is a skewsymmetric matrix such that  $J(x)_{|V}=J$ . Notice that K (trivially) vanishes on the Legendre submanifold generated by  $\phi$ . Furthermore, the dynamics of x given by the contact vector fields  $X_K$  restricted to  $V \cap \mathcal{L}_{\phi} = V \cap \{\phi(x), x, \frac{\partial \phi}{\partial x}(x)\}$  is (12) with  $\Theta(y) = \frac{1}{2}\langle y, Dy \rangle$ .

# III. CONTROL CONTACT SYSTEMS FOR IRREVERSIBLE THERMODYNAMICS

In this section, we shall define control contact systems, in an similar way as input-output Hamiltonian systems [15], [16], [12], with the additional constraint that they satisfy an additional compatibility condition with respect to some Legendre submanifold. This definition is an extension of the definition of conservative systems with ports given in [4]. It is also a completion of the vector fields defined by [10], [14] and recalled in preceding section in the following sense. Firstly we shall consider contact Hamiltonian different from those defining reversible transformations [11]. Secondly we shall augment the contact fields with input vector fields. Therefore, let us first give the definition of the considered class of control contact systems.

Definition 3: A conservative control contact system is defined by :

- a strictly contact manifold  $(\mathcal{M}, \mathcal{E})$  with contact form  $\theta$ .
- a Legendre submanifold  $\mathcal{L}$  of  $(\mathcal{M}, \mathcal{E})$ ,
- an input space  $\mathcal{U} = \mathbb{R}^m$  and input functions  $u_i$ , i = 1 m
- m+1 contact Hamiltonians:  $K_0$  the internal contact Hamiltonian and  $K_j$  the interaction Hamiltonians, satisfying the invariance condition:

$$K_{j|\mathcal{L}} = 0, j = 0, ..., m,$$
 (14)

• the differential equation :

$$\frac{\mathrm{d}}{\mathrm{d}t}(x,x,p) = X_{K_0} + \sum_{j=1}^{m} u_j X_{K_j}.$$
 (15)

It is easy to see, using the theorem 2, that this system leaves invariant the Legendre submanifold.

Hence, in the context of thermodynamic systems, this system may be interpreted as follows. The Legendre submanifold  $\mathcal{L}$  represents the thermodynamical properties of the system. The internal contact Hamiltonian  $K_0$  represents the law giving the fluxes in the closed system due to non-equilibrium conditions in the system (for instance due to heat conduction or chemical reaction kinetics etc...). Finally the interaction Hamiltonian  $K_j$  gives the flows due to the non-equilibrium of the system with its environment. The invariance condition means only that the control system obeys the first principle.

In the first example we shall briefly recall that port Hamiltonian systems form a subclass of the conservative contact systems.

Example 5: In [4], we have shown how, using its adjoint variational systems, a port Hamiltonian system [9], [19] may be lifted as a conservative control contact system (called port conservative system on a contact manifold). Let us recall briefly the definition of a port Hamiltonian system. Consider a n-dimensional differential manifold  $\mathcal{N}$  endowed with a generalized Poisson bracket  $\{.,.\}_{gen}$  (i.e. Jacobi's identities are not necessary satisfied). And denote by  $\Lambda$  its associated pseudo-Poisson tensor. A port Hamiltonian system [9], [18] is defined by a Hamiltonian function  $H_0(x) \in C^{\infty}(\mathcal{N})$ , an input vector  $u(t) = (u_1, \ldots, u_m)^T$  function of t, m input vector fields  $g_1, \ldots, g_m$  on  $\mathcal{N}$ , and the equations:

$$\begin{cases} \dot{x} = \Lambda^{\#}(d_x H_0(x)) + \sum_{i=1}^m u_i(t) g_i(x) \\ y_p^j = \mathcal{L}(g_j) H_0(x), \end{cases}$$
(16)

where  $y_p = (y_p^1, \dots, y_p^m)$  is called the *port output* variable (or *port conjugated variable*). Define the (2n+1)-dimensional thermodynamic state space  $\mathcal{M}$  associated with the base manifold  $\mathcal{N}$  by:

$$\mathcal{M} = \mathbb{R} \times T^* \mathcal{N},\tag{17}$$

endowed with the canonical contact form written in the canonical coordinates  $(x^0, x^i, p_i)$ :

$$\theta = \mathrm{d}x^0 - \sum_{i=1}^n p_i \mathrm{d}x^i,\tag{18}$$

where  $(x^i, p_i)$  are canonical coordinates of the cotangent bundle  $T^*\mathcal{N}$  of the base manifold  $\mathcal{N}$  endowed with the canonical symplectic structure.

Consider the internal contact Hamiltonian

$$K_0 = \Lambda \left( d_x H_0, p \right), \tag{19}$$

and the interaction contact Hamiltonians

$$K_i = i(g_i)(d_x H_0 - p).$$
 (20)

It is clear that the two contact Hamiltonians satisfy the compatibility condition with respect to the Legendre submanifold  $\mathcal{L}_{H_0}$  generated by  $H_0(x)$ . In [4] we have

shown that the restriction to the Legendre submanifold  $\mathcal{L}_{H_0}$  of the conservative system generated by these contact Hamiltonians, gives the state equation of (16). It is interesting to note that the Legendre submanifold is generated by the internal Hamiltonian  $H_0$  of the port Hamiltonian system which has the dimension of energy for models of physical systems, and that the contact Hamiltonians have the dimension of power and are defined by the pseudo-Poisson tensor and the input vector fields.

In this paper, we consider now the case of an autonomous dissipative hamiltonian system defined on  $\mathcal{N}$  by the equation

$$\dot{x} = (J(x) - D(x)) \frac{\partial H_0}{\partial x} , \qquad (21)$$

where D is the symmetric positive definite matrix of friction. Notice that the tensor J-D defines a Leibniz bracket [13]. In order to determine the contact hamiltonian generating this dynamics, we first extend the base manifold as follows:

$$\mathcal{N}_e := \mathbb{R} \times \mathcal{N} , \qquad (22)$$

where we denote by S the coordinate on  $\mathbb{R}$  associated with the entropy. We then define the *extended* thermodynamic phase space

$$\mathcal{T}_e := \mathbb{R} \times T^* \mathcal{N}_e \ni (x^0, x, S, p, T) , \qquad (23)$$

where the conjugated variable to S is the temperature denoted T. This extended thermodynamic phase space is endowed with a canonical contact form  $\theta_e$  defined as previously by

$$\theta_e := \mathrm{d}x^0 - p\,\mathrm{d}x - T\mathrm{d}S \ . \tag{24}$$

We now define the new energy function

$$H_e(x,S) := H_0(x) + T_0 S$$
, (25)

where  $T_0$  is a parameter standing for the constant virtual temperature of the environment, that generates the following Legendre submanifold

$$\mathcal{L}_{H_e} = \left\{ H_e(x, S), x, S, \frac{\partial H_e}{\partial x} = \frac{\partial H_0}{\partial x}, \frac{\partial H_e}{\partial S} = T_0 \right\} (26)$$

of the contact form  $\theta_e$ . Then, we define the contact hamiltonian function

$$K_e := -p^t \left( J(x) - D(x) \right) \frac{\partial H_0}{\partial x} + \frac{T}{T_0} \frac{\partial H_0}{\partial x}^t D(x) \frac{\partial H_0}{\partial x} ,$$
(27)

where the first term is associated with the Leibniz bracket and the second term, arising from the invariance condition (theorem 2), is associated with the dissipation. By construction, this contact hamiltonian  $K_e$  vanishes on  $\mathcal{L}_{H_e}$ . Furthermore, it generates a contact vector fields giving the following dynamics when restricted to  $\mathcal{L}_{H_e}$ 

$$\begin{cases} \dot{x} = (J(x) - D(x)) \frac{\partial H_0}{\partial x} \\ \dot{S} = \frac{1}{T_0} \frac{\partial H_0}{\partial x}^t D \frac{\partial H_0}{\partial x} \end{cases}$$
 (28)

We recognize the dynamics of a dissipative hamiltonian system together with the time variation of the entropy. Notice that this result agrees with the thermodynamic principles: the energy  $H_e$  is conserved and the entropy function is increasing.

Let us now compare the contact hamiltonian (13) presented in [6] and the one we propose in equation (27). First, whereas in (12) the structures matrices are constant, in (27) we take into account x-dependant structure matrices J and D. However, the choice of a contact hamiltonian is quite similar in both cases. Indeed, since one can approximate the potentiel  $\Theta(y)$  by  $\frac{1}{2}\langle y, Dy \rangle$  in a neighborhood V of equilibrium points (see [6]), we still split the contact hamiltonian (13) in two parts: one associated with the Leibniz bracket and the second one with the dissipative term. On the contrary, the thermodynamic spaces as well as the generating potentials of Legendre submanifolds are quite different.

The next example concerns a very classic example of irreversible system, the heat conduction, where the dissipative phenomena is now associated with a physical law of fluxes.

Example 6: Consider a system  $\Sigma$  constituted by two media in contact, only exchanging thermal energy with no volume variation and medium 1 is exchanging a heat flux with the environment.  $\Sigma$  is characterized by its internal energy U, and the pair of conjugated variables  $(S_i, T_i)$  (entropy, temperature) of each medium i. Let  $\mathcal{N} = \mathbb{R}^2 \ni (S_1, S_2)^T$  be the space of the extensive variables and and consider the contact manifold  $(\mathbb{R} \times T^*\mathcal{N})$  endowed with the contact form  $\theta = d\varepsilon - p_i dx^i = dU - T_i dS_i$ . Consider the internal contact Hamiltonian:

$$K_0 = R(p)\Lambda_s \left( dU, p \right), \tag{29}$$

where

$$R(p) = \lambda(p)(1/p_1 - 1/p_2),$$

 $p_i>0$  and  $\lambda$  is the Fourier's conduction coefficient. And consider the interaction contact Hamiltonian

$$K_1 = \frac{\partial U}{\partial S_1} - p_1. \tag{30}$$

It may be shown that the heat conduction system is described by restriction to the Legendre submanifold generated by the energy function U, of the conservative contact control system generated by the contact Hamiltonian (29) (30). It is important to note that, contrary to the lift of the port Hamiltonian system, the internal contact Hamiltonian is no more a bilinear but a nonlinear function of the extensive variable p and dU. This is the key that allow these systems to encompass models arising from Irreversible Thermodynamics.

### IV. PORT CONTACT SYSTEMS AND LOSSLESSNESS

In this section we shall analyze the losslessness properties of conservative control contact systems by defining the conjugated port outputs to the inputs. In the same way as for input-output and port Hamiltonian systems, the differential geometric structure of the system induces the energy balance equation from which the definition of the port conjugated output follows. However, contrary to input-output and port Hamiltonian systems, for conservative control contact systems the energy balance will only be considered on its restriction on the Legendre submanifold (where the thermodynamic properties are satisfied).

Let us first compute the time derivative of a differentiable real function V on  $\mathcal{M}$  with respect to a conservative control contact system (of definition 3). A straightforward calculation, given below in canonical coordinates, leads to the following balance equation:

$$\frac{\mathrm{d}V}{\mathrm{d}t} = K_0 \frac{\partial V}{\partial x^0} + \sum_{i=1}^n p_i \left( \frac{\partial V}{\partial p_i} \frac{\partial K_0}{\partial x^0} - \frac{\partial V}{\partial x^0} \frac{\partial K_0}{\partial p_i} \right) 
+ \sum_{i=1}^n \left( \frac{\partial V}{\partial p_i} \frac{\partial K_0}{\partial x^i} - \frac{\partial V}{\partial x^i} \frac{\partial K_0}{\partial p_i} \right) 
+ \sum_{j=1}^m \left\{ u_j \left[ \frac{\partial V}{\partial x^0} K_j + \sum_{i=1}^n \left( -p_i \frac{\partial V}{\partial x^0} \frac{\partial K_j}{\partial p_i} \right) \right] \right\} 
+ p_i \frac{\partial V}{\partial p_i} \frac{\partial K_j}{\partial x^0} - \frac{\partial V}{\partial p_i} \frac{\partial K_j}{\partial x^i} + \frac{\partial V}{\partial x^i} \frac{\partial K_j}{\partial p_i} \right) \right] \right\} 
= \sum_{j=1}^m u_j \left( \left\{ K_j, V \right\} + V \frac{\partial K_j}{\partial x^0} \right) + \left\{ K_0, V \right\} + V \frac{\partial K_0}{\partial x^0}$$
(31)

This balance equation has a supply rate term which leads to the definition of the V-conjugated output variable:

$$y_V^j = \{K_j, V\} + V \frac{\partial K_j}{\partial x^0}, \tag{32}$$

and a source term defined by :

$$s_V = \{K_0, V\} + V \frac{\partial K_0}{\partial x^0}.$$
 (33)

For a conserved quantity, the source term is expected to be zero. However, as shall be clear in the sequel there is no reason to require it on the entire state space but rather on the Legendre submanifold.

Definition 4: A conserved quantity of a conservative control contact system (definition 3) is a real-valued function V defined on  $\mathcal{M}$  such that

$$s_{V|\mathcal{L}} = 0. (34)$$

Definition 5 ([5]): A port contact system is a control contact system with the additional condition that there exists a generating function U of a Legendre submanifold that is a conserved quantity, completed with the Uconjugated output defined in (32).

In order to motivate the previous definition of conserved quantities, let us first consider some particular cases. First make the following assumptions.

Assumption 1: Assume in the sequel that

1) 
$$\frac{\partial K_i}{\partial x^0} = 0, i = 0, ..., m$$
  
2)  $V = V(x^j), j = 1, ..., n$ 

2) 
$$V = V(x^j), j = 1,..,n$$

The first assumption is quite generally fulfilled for physical systems, as the generation of fluxes in general does not depend explicitly on the energy. The second assumption is more restrictive. However it may be interpreted in the case when one considers V as a generating function of the Legendre submanifold (according to theorem 1), as the expression of the internal energy as a function of the extensive variables of a thermodynamical system. Assume that the assumptions 1 are fulfilled, and let us investigate further the source term  $s_V$  and on the Vconjugated output variable.

Consider firstly under which conditions the source term vanishes. This source term, given in (33), under the assumption 1, reduces to the following expression:

$$s_V = -\frac{\partial V}{\partial x}^T \frac{\partial K_0}{\partial p} \ . \tag{35}$$

Example 7: Consider as a first case the lifted port Hamiltonian system (defined in example 1), and consider as candidate conserved quantity the internal Hamiltonian by setting  $V(x) = H_0(x)$ . Then the source term is written

$$s_V = \frac{\partial H_0}{\partial x}^T \Lambda^\#(\mathrm{d}_x H_0(x)) . \tag{36}$$

Hence the source term is zero on the whole thermodynamic state phase space and the internal Hamiltonian (e.g. the energy of the system) is a conserved quantity on the thermodynamic phase space. It is remarkable that the nullity of the source term  $s_V$  (everywhere on the thermodynamic phase space) is equivalent to the invariance condition of the contact field  $K_{0|\mathcal{L}} = 0$ .

Example 8: Consider now a second case with a generating function given by

$$K_0 = -\langle p, R(x, p)X(x)\rangle, \tag{37}$$

This corresponds to the example 2 of the heat conduction. The source term is now expressed as

$$s_V = R(x, p)i(X)dV + \left(\frac{\partial V}{\partial x}^T \frac{\partial R}{\partial p}\right)i(X)p$$
. (38)

Consider now the function V(x) to be a generating function of the Legendre submanifold  $\mathcal{L}$  (as for instance the internal energy of a thermodynamic system). Then i(X)dV = 0, and the source term reduces to

$$s_V = \left(\frac{\partial V}{\partial x}^T \frac{\partial R}{\partial p}\right) i(X) p .$$
 (39)

which has no reason to be zero on the whole thermodynamic phase space. However it is evident that  $s_V$  vanishes when restricted on the Legendre submanifold  $\mathcal{L}_V$ . It may be noted that the condition that the source term vanishes (on the whole thermodynamic phase space) has no relation with the condition of invariance of the Legendre submanifold:  $\frac{\partial V}{\partial x}^T \frac{\partial K_0}{\partial p} = 0$  for all x in  $\mathcal{M}$ . Let us now consider the definition of V-conjugated

output for a conserved quantity V when the assumptions

1 are satisfied. Under these hypothesis, the expression (32) of port output variables  $y_V^j$  reduces to :

$$y_V^j = -\frac{\partial V}{\partial x}^T \frac{\partial K_j}{\partial p} \ . \tag{40}$$

Consider again first the case of the lift of a port Hamiltonian system on the thermodynamic phase space. For this system, the interaction contact Hamiltonian are  $K_j = \langle \mathrm{d} H_0 - p, g_j \rangle$  and the port conjugated output variables defined in (32) become

$$y_V^j = \frac{\partial H_0}{\partial x}^T g_j = \mathcal{L}(g_j) H_0 . \tag{41}$$

It is remarkable that they correspond precisely to the outputs called *port outputs* defined in (16).

Secondly, consider interaction Hamiltonian functions where the input vector fields may depend on both variables x and p:

$$K_j = \langle dH_0 - p, g_j(x, p) \rangle, \tag{42}$$

and compute the  $H_0$ -conjugated port output :

$$y_V^j = \mathcal{L}(g_j)H_0 + \left(\frac{\partial H_0}{\partial x}^T \frac{\partial g_j}{\partial p}\right) i(g_j)(\mathrm{d}H_0 - p). \tag{43}$$

In this case, the  $H_0$ -conjugated port output variables coincide with the port output variables of (16) only on the Legendre submanifold  $\mathcal{L}_{H_0}$ .

### V. Conclusion

In this paper we have proposed a definition of conservative systems with inputs and outputs defined on contact manifolds. They consist in control contact systems defined in an analogous way to control Hamiltonian systems and generated with respect to a contact structure by an internal and m interaction contact Hamiltonians where m denotes the number of inputs. Conservative contact systems are defined as a subclass of the control contact system generated by contact Hamiltonians which satisfy some compatibility condition with respect to some Legendre submanifold.

In this way one may generalize control and port Hamiltonian systems in order to encompass models arising from Irreversible Thermodynamics. These system also encompass and generalize the systems describing the Reversible Thermodynamics (as for instance reversible transformations of thermodynamical systems). In this case the contact Hamiltonian maybe interpreted as potential functions, having the dimension of power and representing the generation of fluxes arising from non-equilibrium conditions. The Legendre submanifold represents the thermodynamic properties of the systems. And the compatibility condition implies that the systems leaves it invariants which corresponds to satisfying Gibb's relation.

Finally we have investigate the balance equations associated with some invariants of the system. We have

derived a general balance equation for any function, expressed in terms of the contact bracket. This has allowed us to discuss different generating functions. It appears that the conditions of invariance of the Legendre submanifold do not, in general coincide with the conservation of the generating function of the Legendre submanifold. For the lift of port Hamiltonian systems, however, it has been proved that the internal Hamiltonian satisfies a balance equation without source term on the whole thermodynamic phase space.

#### References

- V.I. Arnold. Equations Différentielles Ordinaires. Editions Mir, Moscou, 3-ième édition edition, 1978.
- [2] V.I. Arnold. Mathematical Methods of Classical Mechanics. Springer, ii edition, 1989. ISBN 0-387-96890-3.
- [3] C. Carathéodory. Untersuchungen über die Grundlagen der Thermodynamik. Math. Ann., 67, 1909.
- [4] D. Eberard, B.M. Maschke, and A.J. van der Schaft. Conservative systems with ports on contact manifolds. In *Proc. IFAC World Congress*, Prague, July 2005. to appear.
- [5] D. Eberard, B.M. Maschke, and A.J. van der Schaft. System theory of interconnected port contact systems. In *Proc.* NOLTA Conference, 2005.
- [6] M. Grmela. Reciprocity relations in thermodynamics. *Physica A*, 309:pp. 304–328, 2002.
- [7] R. Herman. Geometry, Physics and Systems. Dekker, New-York, 1973.
- [8] Paulette Libermann and Charles-Michel Marle. Symplectic Geometry and Analytical Mechanics. D. Reidel Publishing Company, Dordrecht, Holland, 1987. ISBN 90-277-2438-5.
- [9] B.M. Maschke and A.J. van der Schaft. Port controlled Hamiltonian systems: modeling origins and system theoretic properties. In proc 3rd NOLCOS, NOLCOS'92, pages 282– 288, Bordeaux, June 1992.
- [10] R. Mrugala. Geometrical formulation of equilibrium phenomenological thermodynamics. Reports on Mathematical Physics, 14(3):419–427, 1978.
- [11] R. Mrugala. On a special family of thermodynamic processes and their invariants. Reports in Mathematical Physics, 46(3):461–468, 2000.
- [12] Henk Nijmeijer and A.J. van der Schaft. Nonlinear Dynamical Control Systems. Springer, New York inc., i edition, 1990. ISBN 0-387-97234-X.
- [13] J.-P. Ortega and V. Planas-Bielsa. Dynamics on Leibniz manifolds. J. of Geometry and Physics, 52:pp. 1–27, 2004.
- [14] J.C. Schon R. Mrugala, J.D. Nulton and P. Salamon. Contact structure in thermodynamic theory. *Reports in Mathematical Physics*, 29(1):109–121, 1991.
- [15] R.W.Brockett. Geometric Control Theory, volume 7 of Lie groups: History, Frontiers and Applications, chapter Control theory and analytical mechanics, pages 1Ű–46. Math.Sci.Press,, Brookline, 1977. C.Martin and R.Herman eds.
- [16] A. van der Schaft. Three Decades of Mathematical System Theory, volume 135 of Lect. Notes Contr. Inf. Sci., chapter System Theory and Mechanics, pages 426Ű–452. Springer, Berlin, 1989.
- [17] A.J. van der Schaft.  $L_2$ -Gain and Passivity Techniques in Nonlinear Control. Springer Communications and Control Engineering series. Springer-Verlag, London, 2nd revised and enlarged edition, 2000. first edition Lect. Notes in Control and Inf. Sciences, vol. 218, Springer-Verlag, Berlin, 1996.
- [18] A.J. van der Schaft and B.M. Maschke. On the Hamiltonian formulation of non-holonomic mechanical systems. Reports on Mathematical Physics, 34(2):225–233, 1994.
- [19] A.J. van der Schaft and B.M. Maschke. The Hamiltonian formulation of energy conserving physical systems with external ports. Archiv für Elektronik und Übertragungstechnik, 49(5/6):362–371, 1995.