# Representation of irreversible systems in a metric thermodynamic phase space $^1$

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Abstract: This paper studies geometric properties of a class of irreversible dynamical systems, referred to in the literature as metriplectic systems. This class of systems, related to generalized (or dissipative) Hamiltonian systems, are generated by a conserved component and a dissipative component and appear, for example, in non-equilibrium thermodynamics. In non-equilibrium thermodynamics, the two potentials generating the dynamics are interpreted as generalized energy and generalized entropy, respectively. Stability and stabilization results for metriplectic systems have been presented in the literature, however, some aspects are still poorly understood, in particular the existence of dynamical invariants such as periodic orbits. In this note, we study the properties of metriplectic systems by considering a lift from the *n*-dimensional state space to a (2n + 1)-dimensional contact space, following an approach introduced in recent years to study irreversible control systems. This lift leads to a deeper geometric characterization of metriplectic systems in the extended space. An example is provided to illustrate the approach proposed in this paper.

Keywords: Nonlinear systems, metriplectic systems, irreversible systems, contact geometry.

## 1. INTRODUCTION

Stability analysis and feedback control design of mechanical systems with no dissipation have had a great impact in nonlinear control theory, see for example (Nijmeijer and van der Schaft, 1990). One reason for that success is the knowledge, in the development of the dynamical equations, of a conserved quantity (i.e., the Hamiltonian function),and the vast amount of available literature on the subject from the field of dynamical systems theory (Arnold, 1989). However, for irreversible systems, the picture is usually not as clear. Dissipative Hamiltonian systems have emerged as a valuable modelling approach for stability analysis and control feedback design (for example damping injection) of systems with dissipation (van der Schaft, 2000; Ortega et al., 2002). However, for chemical processes, since the dynamics is not a priori developed from known potential functions, this approach is difficult for application.

In order to derive potential-driven formulations of (chemical) process dynamics, several researchers considered to start from a thermodynamic point of view, see for example the contributions (Favache et al., 2010; Hoang et al., 2012; Ramirez et al., 2013) and references therein. This approach, based on classical irreversible thermodynamics (de Groot and Mazur, 1962), led to some interesting modelling, stability, and stabilization results with application to chemical reactors. Another approach, proposed originally in (Guay et al., 2012), consisted in recovering a potential-based representation from a given vector field, for example a system of finite-dimensional balance equations, by using Hodge decomposition. By the application of this decomposition approach, it is possible to rewrite a dynamical system as the sum of conserved and nonconserved components. By using the resulting decomposed representation, it is then possible to perform stability analysis and feedback stabilizing control design.

The resulting dynamics can be linked to a class of dynamical systems developed by Morrison (1986) called metriplectic systems, given as

$$\dot{x} = J(x)\nabla^T E(x) - R(x)\nabla^T S(x), \qquad (1)$$

for  $x \in \mathbb{R}^n$  and such that J(x) is antisymmetric  $(J(x) = -J^T(x))$  and R(x) is symmetric positive-definite  $(R(x) = R^T(x) \succ 0)$ . These systems are generated by a conserved quantity E(x), the generalized energy, and a metric quantity S(x), the generalized entropy. Here, we assume that the generating functions E(x) and S(x) are of class  $\mathcal{C}^k(\mathbb{R}^n;\mathbb{R})$ , with  $k \geq 2$ . Stability and geometric properties for systems of the form (1) have been studied extensively (Morrison, 1986; Guha, 2007; Birtea et al., 2007; Birtea and Comănescu, 2009; Hudon et al., 2013a,b, 2014), however it is generally assumed that both functions E(x) and S(x) reach an extremum at the same isolated point, *i.e.*, it is assumed that the system (1) has one isolated equilibrium. In this note, we seek to develop an approach

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to study higher order dynamical invariants, for example periodic orbits.

Metriplectic systems are also interesting from the point of view of non-equilibrium thermodynamic systems, since the so-called GENERIC formulation of thermodynamics, proposed originally in (Grmela and Öttinger, 1997; Öttinger and Grmela, 1997) and reviewed extensively in (Öttinger, 2005), is based on the development of metriplectic systems proposed originally in (Morrison, 1986). Finally, it should be noted that under degeneracy constraints

$$J(x) \cdot \nabla^T S(x) = 0 \tag{2}$$

$$R(x) \cdot \nabla^T E(x) = 0, \tag{3}$$

the dynamics (1) can be re-expressed as dissipative Hamiltonian systems (van der Schaft, 2000; Ortega et al., 2002), *i.e.*, systems of the form

$$\dot{x} = [J(x) - R(x)] \nabla^T H(x),$$

if one pick H(x) to be the free energy at unit temperature, H(x) = E(x) - S(x) (Favache et al., 2010). Obviously, mixed potentials, that is, potentials combining energy and entropy, are known from classical thermodynamics, see for example the availability potential used in (Ydstie and Alonso, 1997) in the context of passive systems theory and control of process systems.

The objective of the present paper is develop an approach to study higher dynamical invariants of metriplectic systems, for example periodic orbits. For conservative systems, such as mechanical systems, this is usually achieved through symplectic geoemtry (Arnold, 1989). In the case of irreversible systems, contact geometry could served the same function. Hence, the proposed approach consists in lifting the *n*-dimensional dynamics to a (2n+1)dimensional contact state-space. This approach has been studied in recent years, starting from the contribution by Eberard et al. (2007) who considered conservative systems with inputs. Stability of conservative port contact systems was considered in (Favache et al., 2009). More recently, this approach was considered in (Ramirez et al., 2013, 2014) for the study of irreversible processes. The idea of using contact geometry in the context of classical (irreversible) thermodynamics is not new, as this space permits to encode thermodynamical constraints, see for example the contributions by Mrugala (1996), Haslach Jr. (1997), Grmela (2002), and (Quevedo, 2007). In (Grmela and Ottinger, 1997), a contact formulation for metriplectic systems (1) under degeneracy constraints (2)-(3) was provided.

The paper is organized as follows. A brief review of elements of contact geometry pertinent to this paper is given in Section 2. The lift of metriplectic systems (1) to the contact phase space is presented in Section 3 with comments on the invariant structure of metriplectic systems based on the contact formulation. An example to illustrated the proposed approach is presented in Section 4. Conclusions and further areas for research are presented in Section 5.

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# 2. CONTACT GEOMETRY FORMALISM

We first briefly summarize the formalism of contact geometry, following the expositions in (Grmela, 2002) and (Ramirez et al., 2013). A complete exposition on the topic can be found in (Arnold, 1989).

Let  $\mathcal{N}$  be a *n*-dimensional manifold. Define the associated contact manifold  $\mathcal{T}$  as  $\mathbb{R} \times T^* \mathcal{N}$  whose elements are denoted  $(x^0, x, p)$ . It has a canonical contact structure defined by t, following the studies presented in (Ramirez et al., 2013), the contact form

$$\theta = dx^0 - \sum_{k=1}^n p_k dx^k.$$
(4)

Definition 1. A one-form  $\theta$  on a 2n + 1-dimensional manifold  $\mathcal{T}$  is a contact form if  $\theta \wedge (d\theta)^n \neq 0$  is a volume form. Then the pair  $(\mathcal{T}, \theta)$  is called a contact manifold.

For a given set of canonical coordinates and any partition  $I \bigcup J$  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

$$x^0 = F - p_J \frac{\partial F}{\partial p_J} \tag{5}$$

$$x^J = -\frac{\partial F}{\partial p_J} \tag{6}$$

$$p_I = \frac{\partial F}{\partial x_I} \tag{7}$$

define a Legendre submanifold of  $\mathbb{R}^{2n+1}$ .

Definition 2. A vector field X on  $(\mathcal{T}, \theta)$  is a contact vector field if and only if there exits a differentiable function  $\rho$  such that

$$\mathcal{L}_X \theta = \rho \theta. \tag{8}$$

To every contact vector field X, one associates the function  $K(x_0, x, p)$ , called the contact Hamiltonian. Conversely, to every function K, there corresponds the contact vector field  $X_K$  given as

$$X_{K} = \left(K - \sum_{k=1}^{n} p_{k} \frac{\partial K}{\partial p_{k}}\right) \frac{\partial}{\partial x^{0}} + \frac{\partial K}{\partial x_{0}} \left(\sum_{k=1}^{n} p_{k} \frac{\partial}{\partial p_{k}}\right) + \sum_{k=1}^{n} \left(\frac{\partial K}{\partial x^{k}} \frac{\partial}{\partial p_{k}} - \frac{\partial K}{\partial p_{k}} \frac{\partial}{\partial x^{k}}\right).$$
(9)

The main contribution of this paper is to consider the "lift" of a *n*-dimensional metriplectic vector field to the contact space, *i.e.*, we will construct a contact Hamiltonian function associated to the system (1) and study the properties of the contact vector field (9).

#### 3. CONTACT LIFT OF METRIPLECTIC SYSTEMS

The idea of "lifting" a *n*-dimensional vector field to the contact phase space was introduced in the context of controlled irreversible systems in (Eberard et al., 2007), and extended in the contributions (Favache et al., 2009, 2010; Ramirez et al., 2013). In particular, in (Ramirez et al., 2013), the drift part of the dynamics was given by

$$\dot{x} = f\left(x, \frac{\partial U}{\partial x}\right),$$

and the contact lift was generated by the contact Hamiltonian function

$$K = \left(\frac{\partial U}{\partial x} - p\right)^T f\left(x, \frac{\partial U}{\partial x}\right)$$

The key argument to suggest such form of contact Hamiltonian is that a contact Hamiltonian defined this way vanishes on the Legendre submanifold generated by U(x). A contact Hamiltonian based on the energy was also used by (Eberard et al., 2007) while an entropy-based lift was employed in (Favache et al., 2010)

In the case of a metriplectic system of the form

$$\dot{x} = J(x)\nabla^T E(x) - R(x)\nabla^T S(x),$$

(without the degeneracy conditions), we select a lift with respect to the conserved quantity E(x). Hence, the contact Hamiltonian function is given by

$$K = \left(\frac{\partial E}{\partial x} - p\right)^T J(x) \nabla^T E(x) - R(x) \nabla^T S(x), \quad (10)$$

and we can construct the contact vector field (9) as:

$$\dot{x}_0 = K - p^T \left( J(x) \nabla E(x) - \nabla^T S(x) \right)$$
(11)

$$\dot{x} = J(x)\nabla^T E(x) - R(x)\nabla^T S(x)$$
(12)

$$\dot{p} = p \cdot \frac{\partial K}{\partial x_0} + \frac{\partial K}{\partial x}.$$
(13)

Remark 3. It should be clear at this point that under the degeneracy conditions (2)-(3), the expression of the contact Hamiltonian would be simplified, *i.e.*, by distributing the terms in K, under degeracy conditions (and the fact that  $\nabla E(x)J(x)\nabla^T E(x) = 0$  would become:

$$\tilde{K} = -p^T \left( J(x) \nabla^T E(x) - R(x) \nabla^T S(x) \right).$$

*Remark 4.* Stability conditions for systems in the contact phase space was studied extensively in (Favache et al., 2009). We leave that part for future investigations.

#### 4. EXAMPLE

To illustrate the approach depicted above, we consider the Fitzhugh–Nagumo reaction equations system, as modeled using a metriplectic formulation in (Xu, 2004). The twodimensional Fitzhugh–Nagumo system is given by

$$\dot{x}_1 = f(x_1) - x_2$$
$$\dot{x}_2 = \sigma x_1 - \gamma x_2,$$

where

$$f(x_1) = -x_1(x_1 - \beta)(x_1 - 1),$$

with  $\sigma$  and  $\gamma$ , some known positive constant. Depending on the value of the parameter  $\beta$  (and its sign), the system trajectories converge to either an isolated equilibrium at the origin or a periodic orbit, see for example Figures 1 for the case of a periodic orbit.

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Fig. 1. Fitzhugh–Nagumo System —  $\sigma=8E-3,~\gamma=1.2E-2,~\beta=-0.139$ 

Since the metriplectic formulation is not unique, there exists multiple formulations of this system (Xu, 2004). Here, we focus on one of those. By setting

$$\begin{split} E(x) &= -\frac{1}{2}\sigma x_1^2 - \beta x_1 x_2 - \frac{1}{2}x_2^2\\ S(x) &= \frac{1}{4}x_1^4 - \frac{\beta + 1}{3}x_1^3 + \frac{\beta + \gamma}{2}x_2^2, \end{split}$$

we have the standard representation

$$\begin{bmatrix} \dot{x}_1\\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1\\ -1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial E}{\partial x_1}\\ \frac{\partial E}{\partial x_2} \end{bmatrix} - \begin{bmatrix} 1 & 0\\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\partial S}{\partial x_1}\\ \frac{\partial S}{\partial x_2} \end{bmatrix}.$$
(14)

It should be noted that in that case, the degeneracy constraints (2)-(3) are not met. With that representation, we can already make the following observation for the case where the origin is an isolated equilibrium (*i.e.*, for  $\beta = 0.139$ ): E(x) reaches a maximum and S(x) reaches a minimum at the origin, which is not true in the case for  $\beta = -0.139$ , as depicted in Figures 2 and 3, respectively.



Fig. 2. Fitzhugh–Nagumo System —  $\sigma=8E-3,\,\gamma=1.2E-2,\,\beta=0.139$ 



Fig. 3. Fitzhugh–Nagumo System —  $\sigma=8E-3,\,\gamma=1.2E-2,\,\beta=-0.139$ 

By inspection of the dynamics alone (or the structure of the potentials), it is not clear why the periodic orbit occurs. However, if one consider the contact Hamiltonian

$$K = \left(\frac{\partial E}{\partial x} - p\right)^T \cdot \left(J(x)\nabla^T E(x) - R(x)\nabla^T S(x)\right),$$

we have

$$K = (-\sigma x_1 - \beta x_2 - p_1)(-\beta x_1 - x_2 - x_1^3 + (\beta_+ 1)x_1^2 + (-\beta x_1 - x_2 - p_2)(\sigma x_1 + \beta x_2 - (\beta + \gamma)x_2), \quad (15)$$

and by inspecting the contact vector field (not shown here), one can see that from a vector field point of view, the dynamics of the dual variables in the contact space are driving the dynamics away for the equilibrium for  $\beta = -0.139$ .

### 5. CONCLUSION

This paper studied dynamical and geometric properties of metriplectic systems by using a lift of the *n*-dimensional state space to a (2n + 1)-dimensional contact space. The main objectives were to develop an approach to study the invariants of metriplectic systems. Following the literature on the study of control systems using contact geometry (Ramirez et al., 2013), future studies would consider feedback control design within the contact geometry framework. From a thermodynamical point of view, the construction of a metric within the contact geometry framework, as suggested for example in (Quevedo, 2007), would also be considered.

#### REFERENCES

- Arnold, V.I. (1989). Mathematical Methods of Classical Mechanics, volume 60 of Graduate Texts in Mathematics. Springer-Verlag, New York, 2nd edition.
- Birtea, P., Boleantu, M., Puta, M., and Tudoran, R.M. (2007). Asymptotic stability for a class of metriplectic systems. *Journal of Mathematical Physics*, 48, 082703.
- Birtea, P. and Comănescu, D. (2009). Asymptotic stability of dissipated Hamilton–Poisson systems. SIAM Journal on Applied Dynamical Systems, 8(3), 967–976.

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- de Groot, S.R. and Mazur, P. (1962). *Non-Equilibrium Thermodynamics*. North-Holland Publishing Company, Amsterdam.
- Eberard, D., Maschke, B.M., and van der Schaft, A.J. (2007). An extension of Hamiltonian systems to the thermodynamic phase space: Towards a geometry of nonreversible processes. *Reports on Mathematical Physics*, 60(2), 175–198.
- Favache, A., Dochain, D., and Maschke, B. (2010). An entropy-based formulation of irreversible processes based on contact structures. *Chemical Engineering Sci*ence, 65, 5204–5216.
- Favache, A., Dos Santos Martins, V., Dochain, D., and Maschke, B. (2009). Some properties of conservative port contact systems. *IEEE Transactions on Automatic Control*, 54, 2341–2351.
- Grmela, M. (2002). Reciprocity relations in thermodynamics. *Physica A*, 309, 304–328.
- Grmela, M. and Öttinger, H.C. (1997). Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Physical Review E*, 56(6), 6620–6632.
- Guay, M., Hudon, N., and Höffner, K. (2012). Representation and control of brayton-moser systems using a geometric decomposition. In Proceedings of the 4th IFAC Workshop on Lagrangian and Hamiltonian Methods for Non Linear Control (LHMNLC 2012), 66-71. Bertinoro, Italy.
- Guha, P. (2007). Metriplectic structure, Leibniz dynamics and dissipative systems. Journal of Mathematical Analysis and Applications, 326, 121–136.
- Haslach Jr., H. (1997). Geometric structgure of the nonequilibrium thermodynamics of homogeneous systems. *Reports on Mathematical Physics*, 39, 147–162.
- Hoang, H., Couenne, F., Le Gorrec, Y., and Dochain, D. (2012). Thermodynamics based stabilization of CSTR networks. In *Proceedings of the 51st IEEE Conference* on Decision and Control, 6352–6357. Maui, HI.
- Hudon, N., Dochain, D., and Guay, M. (2013a). Feedback stabilization of metriplectic systems. In Proceedings of the 2013 IFAC Workshop on Thermodynamics Foundations of Mathematical Systems Theory, 12–17. Lyon, France.
- Hudon, N., Dochain, D., and Guay, M. (2014). Passivity and passive feedback stabilization for a class of mixed potential systems. In *Proceedings of the 19th IFAC* World Congress, 9105–9110. Cape Town, South Africa.
- Hudon, N., Guay, M., and Dochain, D. (2013b). Stability and feedback stabilization for a class of mixed potential systems. In *Proceedings of the 52nd IEEE Conference* on Decision and Control. Firenze, Italy. Submission number 1937.
- Morrison, P.J. (1986). A paradigm for joined Hamiltonian and dissipative systems. *Physica D*, 18, 410–419.
- Mrugala, R. (1996). On a Riemannian metric on contact thermodynamic spaces. *Reports on Mathematical Physics*, 38(3), 339–348.
- Nijmeijer, H. and van der Schaft, A. (1990). Nonlinear Dynamical Control Systems. Springer-Verlag, New York, NY.
- Ortega, R., van der Schaft, A., Maschke, B., and Escobar, G. (2002). Interconnection and damping assignment passivity-based control of port-controlled Hamiltonian systems. *Automatica*, 38, 585–596.

- Öttinger, H.C. (2005). Beyond Equilibrium Thermodynamics. Wiley, Hoboken, NJ.
- Öttinger, H.C. and Grmela, M. (1997). Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism. *Physical Review E*, 56(6), 6633–6655.
- Quevedo, H. (2007). Geometrothermodynamics. Journal of Mathematical Physics, 48, 013506.
- Ramirez, H., Le Gorrec, Y., and Maschke, B. (2014). Interconnection and damping assignment - passivity based control of irreversible port Hamiltonian systems. In *Proceedings of the 19th IFAC World Congress*, 9111– 9116. Cape Town, South Africa.
- Ramirez, H., Maschke, B., and Sbarbaro, D. (2013). Irreversible port-Hamiltonian systems: A general formulation of irreversible processes with application to the CSTR. *Chemical Engineering Science*, 89, 223–234.
- van der Schaft, A. (2000).  $L_2$ -gain and Passivity Techniques in Nonlinear Control. Communications and Control Engineering Series. Springer-Verlag, London, 2nd edition.
- Xu, B. (2004). Metriplectic Representation of Finite Dimensional Dynamical Systems. Ph.D. thesis, Portland State University.
- Ydstie, B. and Alonso, A. (1997). Process systems and passivity via the Clausius–Planck inequality. Systems and Control Letters, 30, 253–264.