Port contact Hamiltonian systems for Irreversible systems

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Introduction and motivation

Introduction and motivation

Context and motivation

Use physical invariants and coupling in the :

1. physically-based modelling making use of physical invariants
2. physically-based control design : design control Lyapunov functions using physical invariants
3. simultaneous design of process an control using physical analogy of the controller or the closed-loop system

Competing formulations for physical systems' dynamics and control

Competing formulations for open physical systems

Mechanical systems' dynamics and control

The structure of the dynamical equations may be **related to Mathematical Physics : Lagrangian and Hamiltonian systems** defined on T^*Q, Q configuration manifold and augmented with input-output maps.

- R.W.Brockett, *Control theory and analytical mechanics*,in **Geometric Control Theory**, C.Martin and R.Herman eds., pp.1–46, Vol. VII of Lie groups: History, Frontiers and Applications, Math.Sci.Press, Brookline, 1977
- A.J. van der Schaft, **System Theoretic Description of Physical Systems**, CWI Tracts, Mathematisch Centrum, Amsterdam, 1984
- A.J. van der Schaft, *System Theory and Mechanics*, in **Three Decades of Mathematical System Theory**, H.Nijmeijer and J.M.Schumacher eds., Lect. Notes Contr. Inf. Sci.,Vol.135, pp. 426–452, Springer, Berlin, 1989
- J.E.Marsden, **Lecture Notes on Mechanics**, London Math. Soc. Lecture Notes Series, 174, Cambridge Un. Press, Great Britain, 1992

Network systems' dynamics and control

For electrical circuits: Port/standard Hamiltonian systems, pseudo-gradient systems: Kirchoff's laws and n-port elements

- Hamiltonian systems
  - G.M. Bernstein and M.A. Lieberman, "*A method for obtaining a canonical Hamiltonian for nonlinear LC circuits,* **IEEE Trans. on Circuits and Systems**, CAS–35, 3, 411–420,1989
  - B.M. Maschke, A.J. van der Schaft and P.C. Breedveld, "*An intrinsic Hamiltonian formulation of network dynamics: non–standard Poisson structures and gyrators*", **Journal of the Franklin Institute**, Vol. 329, n. 5, pp. 923–966, 1992
- Brayton-Moser equations (or pseudo- gradient systems)
  - R.K. Brayton and J.K. Moser, "*A Theory of Nonlinear Networks–I and II*", **Quartely of Applied Mathematics**, Vol.22, nº1, pp.1–33, April 1964 and nº2, pp.81–104, July 1964
  - S. Smale, "*On the Mathematical Foundations of Electrical Circuit Theory*", **J. of Differential Geometry**, Vol.7, pp.193–210, 1972
  - D. Jeltsema, R. Ortega, J.M.A. Scherpen, *On passivity and power-balance inequalities of nonlinear RLC circuits*, **IEEE Trans. Circuits and Systems**

Dissipative systems' dynamics and control

For electro-mechanical systems with dissipation : controlled Lagrangian and Hamiltonian systems with dissipation, dissipative port Hamiltonian systems

- A.J. van der Schaft, *System Theory and Mechanics*, in **Three Decades of Mathematical System Theory**, H.Nijmeijer and J.M.Schumacher eds., Lect. Notes Contr. Inf. Sci.,Vol.135, pp. 426–452, Springer, Berlin, 1989
- van der Schaft, A., Maschke, B., The Hamiltonian formulation of energy conserving physical systems with external ports. Arch. für Elektronik und Übertragungstech. 49, 362–371, 1995

For chemical engineering: gradient systems, GENERIC systems, irreversible port contact systems

- Otero-Muras, I., Szederkényi, G., Alonso, A.A., Hangos, K.M., Local dissipative Hamiltonian description of reversible reaction networks. Syst. ControlLett. 57, 554–560, 2008.
- H., Grmela, M., Dynamics and thermodynamics of complex fluids. ii. Illustrations of a general formalism. Phys. Rev. E56, 6633–6655, 1997..

Contact geometry for open thermodynamic systems

For thermodynamical systems one has to consider simulataneously the energy balance and the entropy balance equation with the irreversible entropy creation term. This is not encompassed in (dissipative) Hamiltonian systems.
The objective is to develop a similar control theory for irreversible Thermodynamic systems :

1. intrinsic structure of state space is contact manifold
2. the dynamics is described by contact vector fields.

inspired by work of M. Grmela and R. Mrugała

The geometry of Thermodynamics

The geometry of Thermodynamics

Thermodynamical properties

Thermodynamical properties

Equilibrium Thermodynamics

Equilibrium Thermodynamics characterizes the thermodynamical properties of matter (extremely diverse and complex) : constitutive remations with respect to energy (or any thermodynamical potenetial function)

In general there are not given by a real-valued function, like in mechanics but given in the Thermodynamical Phase Space consisting of :

1. $n+1$ extensive variables denoted $(x^0, x^1, \dots, x^n)$
2. n intensive variables denoted $(p_1, \dots, p_n)$

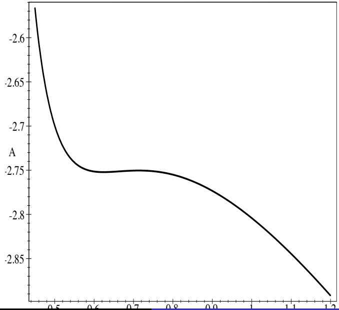
by Gibbs' relation : $dx^0 = \sum_{i=1}^{n} p_i \, dx^i$

This gives **a canonical geometric structure to thermodynamial systems called *contact structure***.

Thermodynamical properties : Gibbs' fundamental relation

They are defined on $n+1$-dimensional ***space of extensive variables*** $\mathscr{N} \sim \mathbb{R}^{n+1}$:

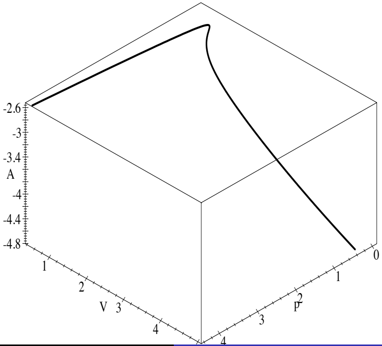
1. energy $x^0 \in \mathbb{R}$
2. remaining extensive variables $x \in \mathbb{R}^n$
3. the ***fundamental equation***: $x^0 = U(x)$



Thermodynamical properties : Gibbs' equations

Thermodynamic Phase space $\mathscr{T} \sim \mathbb{R}^{2n+1}$, the space of 1-jets over $\mathscr{N}$:

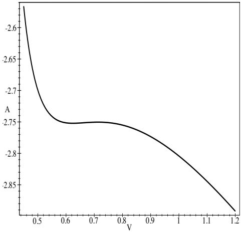
- additional *intensive variables* $p \in \mathbb{R}^n$
- ***Gibb's relation***: $dx^0 = \sum_{i=1}^n p_i \, dx^i$

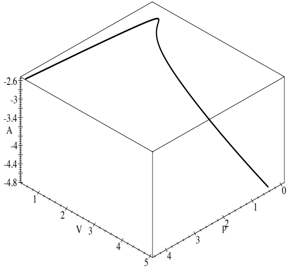


Thermodynamical properties

For a simple Thermodynamic System:

- extensive variables: energy U, entropy S, volume V, number of moles N
- intensive variables: temperature T, pressure P, chemical potential μ
- Gibbs' relation $dU = TdS + (-P)dV + \mu dN$





Contact geometry and Thermodynamics

Contact geometry and Thermodynamics

Intrinsic definitions : contact structure

Definition

A contact structure on a manifold $\mathscr{M}$ is determined by a 1-form θ of constant class $(2n+1)$. The pair $(\mathscr{M}, \theta)$ is then called a *contact manifold*, and θ a *contact form*.

According to Darboux's theorem there exists a set of *canonical coordinates* $(x_0, x, p) \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n$ of $\mathscr{M}$ where the contact form θ is given by : $\theta = dx_0 - \sum_{i=1}^n p_i dx_i$

Definition

The Reeb vector field E associated with the contact form θ is the unique vector field satisfying $i_E \theta = 1 \quad \text{and} \quad i_E d\theta = 0$

where i_E denotes the contraction by the vector field E of differential forms

The geometry of Equilibrium Thermodynamics

some references

1. C.Carathéodory, Untersuchungen über die Grundlagen der Thermodynamik, **Math. Ann.**, 1909
2. Gibbs, J.W.,**Collected Works : I : Thermodynamics**, Longmans, 1928
3. Herman, R., **Geometry, Physics and Systems**, Dekker, 1973
4. R. Mrugała, Geometrical formulation of equilibrium phenomenological Thermodynamics, **Reports on Mathematical Physics**, 1978

Thermodynamical properties: a geometric perspective

The solutions to a Pfaffian equation :

$$\theta|_{\mathscr{L}} = \mathrm{d}x^0 - p_i \mathrm{d}x^i\big|_{\mathscr{L}} = 0 \tag{1}$$

are given by a
Legendre submanifold $\mathscr{L}$ which is defined, in a given set of canonical coordinates $(x^0, x^1, \dots, x^n, p_1, \dots, p_n)$ by:

- a partition $I \cup J$ of the set of indices $\{1, \dots, n\}$
- a **differentiable function** $F(x^I, p_J)$ of n variables, $i \in I, j \in J$
- and the equations:

$$x^0 = F - p_J \frac{\partial F}{\partial p_J}, \quad x^J = -\frac{\partial F}{\partial p_J}, \quad p_I = \frac{\partial F}{\partial x^I}$$

Pure monoatomic perfect gas

generated by the free energy

1. the thermodynamical phase space:
   energy $x^0 = U$, extensive variables: $x^i = S, V, N$,
   intensive variables: $p_i = T, P, \mu$
2. Gibbs' form $\theta = d\,U - T\,d\,S + P\,d\,V - \mu\,d\,N$
3. the Legendre submanifold is generated by the ***free energy***:
   $G(T, -P, N) =$
   $5/2NRT(1 - ln(T/T_0)) - NT(s_0 - R\,ln(P/P_0))$ where R is the constant of perfect gases and T_0, P_0, s_0 are constants:

$$\begin{cases} U(T,-P,N) = \dfrac{3}{2}NRT \\ S(T,-P,N) = Ns = Ns_0 + \dfrac{5}{2}NRln(\dfrac{T}{T_0}) - NRln(\dfrac{P}{P_0}) \\ V(T,-P,N) = \dfrac{NRT}{P} \\ \mu(T,-P,N) = \dfrac{5}{2}RT - Ts \end{cases}$$

Reversible transformations

Reversible transformations

Contact vector fields: definition

Definition

A (smooth) vector field X on the contact manifold $\mathscr{M}$ is a contact vector field with respect to a contact form θ if and only if there exists a smooth function $\rho \in C^\infty(\mathscr{M})$ such that $L_X\theta = \rho\theta$,

where $L_X\cdot$ denotes the Lie derivative with respect to the vector field X.

Theorem

The map $\Phi(X) = i_X\theta$ defines an isomorphism from the vector space of contact vector fields in the space of smooth real functions on the contact manifold.

The function $K = \Phi(X)$ is called contact Hamiltonian
the function ρ is $\rho = i_E dK$ where E is the Reeb vector field.

Contact vector field in coordinates

Theorem

In a set of canonical coordinates $(x^0, x^1, \ldots, x^n, p_1, \ldots, p_n)$, the contact vector field is expressed by:

$$X_K(x) = \begin{bmatrix} K \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & -p^\top \\ 0 & 0 & -I_n \\ p & I_n & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial K}{\partial x_0} \\ \frac{\partial K}{\partial x} \\ \frac{\partial K}{\partial p} \end{bmatrix}$$

where I_n denotes the $n \times n$ identity matrix.

Decomposition of vector fields $(\mathscr{M}, \theta)$

The tangent bundle $T\mathscr{M}$ may be decomposed into

$$T\mathscr{M} = \ker d\theta \oplus \ker\theta \tag{2}$$

where $\ker d\theta$, called *vertical bundle* , is of rank 1 and is generated by the Reeb vector field and $\ker\theta$, called *horizontal bundle*, is of rank $2n$.

Every vector field X on $\mathscr{M}$ may be decomposed in a unique way into

$$X = \underbrace{(i_X\theta)\,E}_{\in\ker d\theta} + \underbrace{(X - (i_X\theta)\,E)}_{=\mathscr{H}(X)\in\ker\theta=\mathscr{C}} \tag{3}$$

where $(i_X\theta)\,E$ is horizontal and $(X - (i_X\theta)\,E)$ is horizontal and is denoted by $\mathscr{H}(X)$.

Decomposition of contact vector fields $(\mathscr{M}, \theta)$

$$\Phi^{-1}(f) = X_f = f\,E + \theta^{\sharp}\left(df - (i_E df)\,\theta\right) \tag{4}$$

where $f\,E$ is the vertical and $\theta^{\sharp}\left(df - (i_E df)\,\theta\right)$ is the horizontal components of the contact vector field.
Note that if the contact Hamiltonian f is is a first integral of the Reeb vector field (i.e. satisfies $i_E df = 0$ or in other words, it differential df is semi-basic), then

$$X_f = f\,E + \theta^{\sharp}(df)$$

and leaves invariant the contact form and is called *strict contact vector field.*

Contact vector fields leaving invariant a Legendre submanifold

Consider a Legendre submanifold $\mathscr{L}$

Theorem

[Mrugała, 1991] Then X_K is tangent to $\mathscr{L}$ if and only if K is identically zero on $\mathscr{L}$:

$$\mathscr{L} \subset K^{-1}(0)$$

This characterizes contact fields which leave invariant some thermodynamical properties.

For instance: reversible thermodynamic transformations are generated by the state equations.

Reversible transformation of a perfect gas

Consider as contact Hamiltonian function the **state equation**

$$K(U, S, V, B, -T, P, -\mu) = U - (3/2)NRT$$

The associated contact vector field is :

$$X_K = U\frac{\partial}{\partial U} + T\frac{\partial}{\partial T} + P\frac{\partial}{\partial P} + \left(\mu - \frac{3}{2}RT\right)\frac{\partial}{\partial \mu} + \frac{3}{2}NR\frac{\partial}{\partial S} + 0\frac{\partial}{\partial V} + 0\frac{\partial}{\partial N}$$

Thus the integral curves of X_K are isochore reversible transformations of the closed system

$$U(t) = U_0 e^t, \quad T(t) = T_0 e^t, \quad P(t) = P_0 e^t, \quad \mu(t) = \mu_0 e^t - \tfrac{3}{2} R T_0 e^t,$$
$$S(t) = S_0 + \tfrac{3}{2} N_0 R t, \quad V(t) = V_0, \quad N(t) = N_0$$

Since $\mathscr{L} \subset K^{-1}(0)$, X_K is tangent to $\mathscr{L}$:

the thermodynamical properties of the ideal gas are preserved along the integral curves.

The dynamics of Irreversible Thermodynamics

The dynamics of Irreversible Thermodynamics

The geometry of Irreversible Thermodynamics

Irreversible Thermodynamics deals with systems subject to irreversible phenomena

1. mass transport through diffusion
2. heat transport through conduction ...

due to non-equilibrium condition between subsystems or with the environment.

We shall use contact vector fields naturally defined on contact structure for a geometrically consistent definition of the dynamic equations of irreversible, open processes.

Conservative system on a contact manifold

A conservative system on a contact manifold is defined by:

1. a strictly contact manifold $\mathscr{M}$ with contact form θ (the Thermodynamic Phase Space)
2. a Legendre submanifold $\mathscr{L}$ (the Thermodynamic properties)
3. a contact Hamiltonian K_0 (the potential generating the fluxes) and satisfying the invariance condition:

$$K|_{\mathscr{L}} = 0$$

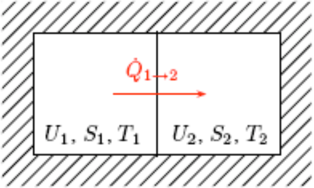
4. the differential equation: $\frac{d\tilde{x}}{dt} = X_{K_0}$

Two cells exchanging heat

Two cells exchanging heat

Two cells exchanging heat

Two cells exchanging heat : the paradigm of coupled entropy balance equations



Thermodynamic model given by Gibbs' relation : $dU_i = T_i \, dS_i$ where $T_i = \frac{\partial U_i}{\partial S_i}(S_i), \; i = 1, 2$

Heat flux due to conducting wall : $\dot{Q}_{1\to 2} = \lambda \, (T_1 - T_2)$ with λ the heat conduction coefficient

Continuity of heat flux : $\dot{Q}_{1\to 2} = -T_1 \frac{dS_i}{dt} = T_2 \frac{dS_2}{dt}$

Dynamics of the 2 cells lift to a contact sytem

Thermodynamic phase space has the coordinates:

1. energy x^0
2. entropies $x^i \in \mathcal{N} = \mathbb{R}^2$
3. temperatures $p_i \in T_S^*\mathcal{N} \approx \mathbb{R}^2$

with contact form $\theta = dx^0 - p_i dx^i$

a Legendre submanifold $\mathscr{L} \ni \left(U, S^i, T_i\right)$ generated by $U(S)$

the contact Hamiltonian $K_0(p, T) = -R(T(x), p)p^\top J_s T(x)$, with $R(T(x), p) = \lambda \left(\frac{p_1 - p_2}{T_1 T_2}\right)$
satisfies the invariance condition and **has the dimension of power**.

Dynamics of the 2 cells on the Thermodynamic Phase Space

The energy coordinate dynamics:

$$\frac{dx^0}{dt} = \lambda \left(\frac{p_1 - p_2}{T_1 T_2} \right) \left(\frac{\partial S}{\partial x}^\top Jp \right) \underbrace{\left(p^\top J \frac{\partial U}{\partial x} \right)}_{|_{\mathscr{L}} = 0} \tag{5}$$

The entropy coordinate dynamics:

$$\frac{dx_i}{dt} = \lambda \left(\frac{p_1 - p_2}{T_1 T_2} \right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \left[\underbrace{\left(p^\top J \frac{\partial U}{\partial x} \right)}_{|_{\mathscr{L}} = 0} \frac{\partial S}{\partial x} + \underbrace{\left(\frac{\partial S}{\partial x}^\top Jp \right)}_{= p_1 - p_2} \frac{\partial U}{\partial x} \right] \tag{6}$$

The temperature coordinate dynamics :

$$\frac{dp_i}{dt} = - \underbrace{\left(p^\top J \frac{\partial U}{\partial x} \right)}_{|_{\mathscr{L}} = 0} \frac{\partial}{\partial x} \left[\lambda \left(\frac{p_1 - p_2}{T_1 T_2} \right) \left(\frac{\partial S}{\partial x}^\top Jp \right) \right] + \lambda \left(\frac{p_1 - p_2}{T_1 T_2} \right) \underbrace{\left(\frac{\partial S}{\partial x}^\top Jp \right)}_{= p_1 - p_2} \frac{\partial^2 U}{\partial x^2}(x) Jp \tag{7}$$

Dynamics of the 2 cells on the Legendre submanifold

The energy balance equation:

$$\left.\frac{dx^0}{dt}\right|_{\mathscr{L}} = \frac{dU}{dt} = 0 \tag{8}$$

The **local energy balance** (expressed on temperatures) :

$$\left.\frac{dp_i}{dt}\right|_{\mathscr{L}} = \frac{dT_i}{dt} = \begin{pmatrix} -{C_V}_1^{-1}\lambda(T_1 - T_2) \\ {C_V}_2^{-1}\lambda(T_1 - T_2) \end{pmatrix} \tag{9}$$

The entropy balance equation :

$$\left.\frac{dx_i}{dt}\right|_{\mathscr{L}} = \frac{dS_i}{dt} = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} T_1 \\ T_2 \end{pmatrix} \tag{10}$$

Controlled contact systems

Controlled contact systems

Controlled conservative contact system

Definition

A *control contact system* is defined by:

1. a contact manifold $\mathbb{R}^{2n+1}$ with contact form θ
2. a Legendre submanifold $\mathfrak{L}$
3. $m+1$ a contact Hamiltonians: K_0 internal and K_j **interaction Hamiltonian**

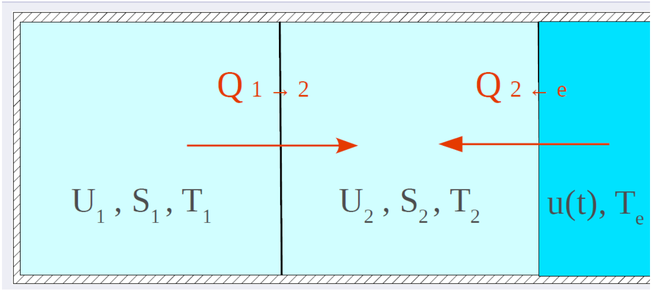
   satisfying the invariance condition:

$$K_{j_{|\mathfrak{L}}} = 0\,, j = 0, \ldots, m$$

4. the differential equation: $\dot{\tilde{x}} = X_{K_0} + \sum_{j=1}^{m} u_j X_{K_j}$

2 cells with thermostat

Two simple thermodynamic systems 1 and 2 interact through a heat conducting conducting wall and system 2 interacts with a thermostat at temperature $T_e = u$.



2 cells with thermostat: pseudo-Hamiltonian formulation

The control pseudo PHS is defined by:

$$\dot{x} = R(x, T(x))J\frac{\partial U}{\partial x}(x) + W + g(T)u$$

where $W + g(T)u$ represent the external "forces" is then :

$$\begin{aligned}
\begin{bmatrix}\dot{S}_1\\ \dot{S}_2\end{bmatrix} &= \lambda\left(\frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{\frac{\partial U}{\partial S_1}}\right)\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial U}{\partial S_1}\\ \frac{\partial U}{\partial S_2}\end{bmatrix} + \lambda_e\begin{bmatrix}0\\ \frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{u}\end{bmatrix}u\\
&= \underbrace{\lambda\left(\frac{1}{\frac{\partial U}{\partial S_2}} - \frac{1}{\frac{\partial U}{\partial S_1}}\right)}_{R=R(x,T(x))}\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial U}{\partial S_1}\\ \frac{\partial U}{\partial S_2}\end{bmatrix} + \underbrace{-\lambda_e\left[\begin{smallmatrix}0\\1\end{smallmatrix}\right]}_{=W} + \underbrace{\frac{\lambda_e}{T_2}\left[\begin{smallmatrix}0\\1\end{smallmatrix}\right]}_{=g} u,
\end{aligned}$$

2 cells with thermostat as a port contact system

- Thermodynamic phase space has the coordinates: energy x^0, entropies $x^i \in \mathscr{N} = \mathbb{R}^2$, temperature $p_i \in T_S^*\mathscr{N} \approx \mathbb{R}^2$
- with contact form $\theta = dx^0 - p_i dx^i$
- a Legendre submanifold $\mathscr{L} \ni \left(U, S^i, T_i\right)$ generated by $U(S)$
- the internal contact Hamiltonian: $K_0\,(p,\,T) = -\lambda\left(\frac{p_1-p_2}{T_1\,T_2}\right)p^\top J_s\,T(x),$
- **the control Hamiltonian:**

$$K_c(x,p) = \left(1 - \frac{p_2}{T_2}\right)\lambda_e\left(T_e - p_{1\,2}\right) \tag{11}$$

2 cells with thermostat: contact system in coordinates

The energy coordinate dynamics:

$$\frac{dx^0}{dt} = \lambda \left(\frac{p_1 - p_2}{T_1 T_2} \right) \left(\frac{\partial S}{\partial x}^\top Jp \right) \underbrace{\left(p^\top J \frac{\partial U}{\partial x} \right)}_{|_{\mathscr{L}}=0} + \lambda_e \left(T_e - p_{12} \right) \quad (12)$$

The entropy coordinate dynamics :

$$\frac{dx_i}{dt} = \lambda \left(\frac{p_1 - p_2}{T_1 T_2} \right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \left[\underbrace{\left(p^\top J \frac{\partial U}{\partial x} \right)}_{|_{\mathscr{L}}=0} \frac{\partial S}{\partial x} + \underbrace{\left(\frac{\partial S}{\partial x}^\top Jp \right)}_{=p_1 - p_2} \frac{\partial U}{\partial x} \right] + \begin{pmatrix} 0 \\ \frac{1}{T_2} \end{pmatrix} \lambda_e \left(T_e - p_{12} \right) \quad (13)$$

The temperature coordinate dynamics :

$$\left. \frac{d{x^1}_i}{dt} \right|_{\mathscr{L}} = \frac{dS_i}{dt} = \lambda \left(\frac{1}{T_2} - \frac{1}{T_1} \right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} T_1 \\ T_2 \end{pmatrix} + \begin{pmatrix} 0 \\ \lambda_e \left(\frac{1}{T_2} - \frac{1}{T_e} \right) T_e \end{pmatrix} \quad (14)$$

2 cells with thermostat: restriction to the Legendre submanifold

The **energy balance equation**:

$$\left.\frac{dx^0}{dt}\right|_{\mathscr{L}} = \frac{dU}{dt} = \lambda_e\left(T_e - T_2\right) \tag{15}$$

The entropy balance equation :

$$\left.\frac{d{x^1}_i}{dt}\right|_{\mathscr{L}} = \frac{dS_i}{dt} = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right)\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} T_1 \\ T_2 \end{pmatrix} + \begin{pmatrix} 0 \\ \lambda_e\left(\frac{1}{T_2} - \frac{1}{T_e}\right) T_e \end{pmatrix} \tag{16}$$

The local energy balance (expressed on temperatures) :

$$\left.\frac{d{p_1}_i}{dt}\right|_{\mathscr{L}} = \frac{dT_i}{dt} = \begin{pmatrix} -{C_V}_1^{-1}\lambda(T_1 - T_2) \\ {C_V}_2^{-1}\lambda(T_1 - T_2) \end{pmatrix} + \begin{pmatrix} 0 \\ {C_V}_2^{-1}\lambda_e(T_e - T_2) \end{pmatrix} \tag{17}$$

The CSTR

The Continuous Stirred Tank Reactor

Continuous Stirred Tank Reactor

Assume a chemical reaction in a CSTR with the following reversible reaction scheme

$$\nu_1 A_1 + \ldots + \nu_l A_l \rightleftharpoons \nu_{l+1} A_{l+1} + \ldots + \nu_m A_m, \qquad m > l \geq 1.$$

and assume V the volume in the reactor as well as the pressure P are constant.

The contact formulation is obtained by lifting the Irreversible Port Hamiltonian formulation

$$\dot{x} = R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W(x, F_e) + g\frac{Q}{T} * \tag{18}$$

on the Thermodynamic phase space $\mathbb{R}^{2n+1} \ni (x_0, x, p)$ with $x = [\mathbf{n}, S]^\top$.

CSTR: Thermodynamic Properties

The thermodynamic properties of the mixture in the reactor (with assumption of constant volume and pressure) may be defined by the Legendre submanifold of the TPS $\mathbb{R}^{2n+1} \ni (x_0, x, p)$, generated by the internal energy function $U(\mathbf{n}, S)$

$$\mathscr{L}_U : \begin{cases} x_0 = U(\mathbf{n}, S) \\ x = [\mathbf{n}, S]^\top \\ p = [\mu(\mathbf{n}, S),\ T(\mathbf{n}, S)]^\top \end{cases} \tag{19}$$

CSTR: internal contact Hamiltonian

Internal contact Hamiltonian

$$K_0 = -p^\top R_e\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}, p\right) J \frac{\partial U}{\partial x}(x)$$

with

$$R_e\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}, p\right) = \frac{r(\mathscr{A}_f(\mu), \mathscr{A}_r(\mu), T)V}{T(x)\mathscr{A}(\mu)} \mathscr{A}(p). \tag{20}$$

Virtual energy balance due to chemical reaction

$$r(\mathscr{A}_f(\mu), \mathscr{A}_r(\mu), T)V\left[\mu^\top \mathscr{A}(p) - p^\top \mathscr{A}(\mu)\right]$$

CSTR: control contact Hamiltonian

Control contact Hamiltonian

$$K_c = \left(\frac{\partial U}{\partial x} - p\right)^\top \left[W\left(x, \frac{\partial U}{\partial x}, p\right) + g\frac{Q}{T}\right] \text{ with}$$

$$W\left(x, \frac{\partial U}{\partial x}\right) = \begin{bmatrix} F_{e1} - F_{s2}\left(x, \frac{\partial U}{\partial x}\right) \\ \vdots \\ F_{em} - F_{sm}\left(x, \frac{\partial U}{\partial x}\right) \\ \frac{1}{T}\sum_{i=1}^m \left(F_{ei}s_{ei} - F_{si}\left(x, \frac{\partial U}{\partial x}\right) s_i\left(x, \frac{\partial U}{\partial x}\right)\right) \end{bmatrix},$$

- mass exchange with the environment

$$\sum_{i=1}^m (\mu_i - p_i)\left(F_{ei} - F_{si}\left(x, \frac{\partial U}{\partial x}\right)\right)$$

- (thermal) energy exchange with environment

$$(T - p_S)\left(\sum_{i=1}^m \left(F_{ei}s_{ei} - F_{si}(x,p)\, s_i\left(x, \frac{\partial U}{\partial x}\right)\right) + \frac{Q}{T}\right)$$

Some references

1. R. Mrugała. *On a special family of thermodynamic processes and their invariants*. **Reports in Mathematical Physics**, 46(3) :461–468, 2000
2. Grmela, M., *Reciprocity relations in thermodynamics*, **Physica A**, 2002
3. D. Eberard, B.M. Maschke, and A.J. van der Schaft. *An extension of pseudo-Hamiltonian systems to the thermodynamic space : towards a geometry of non-equilibrium thermodynamics*. **Reports on Mathematical Physics**, 60(2) :175–198, 2007
4. H. Ramırez Estay , B. Maschke and D. Sbarbaro, *Irreversible port-Hamiltonian systems : A general formulation of irreversible processes with application to the CSTR*, **Chemical Engineering Science**, Volume 89, pp. 223-234 15 February 2013

Variational contact systems

Control contact systems: a variational approach

Alternative definition of contact vector fields

Definition

A contact vector field X_K generated by the Hamiltonian function $K(\tilde{x})$ is the unique vector field satisfying

$$\begin{aligned} i_X \theta &= K \\ i_X d\theta &= -dK(\mathscr{H}(X)) = -(dK - (i_E dK)\theta) \end{aligned} \tag{21}$$

In a set of canonical coordinates $(x^0, x^1, \dots, x^n, p_1, \dots, p_n)$, the contact vector field is expressed by:

$$X_K(x) = \begin{bmatrix} K \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & -p^\top \\ 0 & 0 & -I_n \\ p & I_n & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial K}{\partial x_0} \\ \frac{\partial K}{\partial x} \\ \frac{\partial K}{\partial p} \end{bmatrix}$$

Variational contact systems [Merker et al. 2013]

A *variational control contact system* on $(\mathscr{M}, \theta)$, is defined by
(i) *output variables* defined by the vector bundle $E \ni y$ over$\mathscr{M}$ with flat covariant derivative ∇
(ii) a bundle map $A : T^*\mathscr{M} \to E$ with $A(\theta) = 0$
(ii) *conjugated input variables* is the dual bundle $E^* \ni u$ over$\mathscr{M}$
(iii) *input map* defined by the adjoint bundle map $A^* : E^* \to T\mathscr{M}$
(iv) *internal contact Hamiltonian function* $K_0(\tilde{x})$
and the dynamical system $\frac{d\tilde{x}}{dt} = X(\tilde{x}, u, y)$ with the unique vector field $X(\tilde{x}, u, y)$ satisfying

$$\begin{aligned} i_{(X - A^* u)} d\theta + dK_0 = 0 \\ \theta(X) = i_X \theta = K_0 + \langle u, y \rangle \end{aligned} \qquad (22)$$

Reminder on decomposition of vector fields

The tangent bundle $T\mathscr{M}$ may be decomposed into

$$T\mathscr{M} = \ker d\theta \oplus \ker \theta$$

where $\ker d\theta$, called *vertical bundle* , is of rank 1 and is generated by the Reeb vector field
$\ker \theta$, called *horizontal bundle*, is of rank $2n$.
Every vector field X on $\mathscr{M}$ may be decomposed in a unique way into

$$X = (i_X\theta)\,E + (X - (i_X\theta)\,E)$$

where $(i_X\theta)\,E \in \ker d\theta$ is vertical and
$(X - (i_X\theta)\,E) = \mathscr{H}(X) \in \ker \theta = \mathscr{C}$ is horizontal with respect to the contact form θ .

Variational contact systems as explicit nonlinear system (1)

Using the decomposition of the tangent manifold $T\mathscr{M} = \ker d\theta \oplus \ker \theta$, the variational contact system is

$$\begin{aligned} X(\tilde{x}, u, y) &= \underbrace{(i_X\theta)\,E}_{\in \ker d\theta} + \underbrace{(X - (i_X\theta)\,E)}_{=\mathscr{H}(X)\in\ker\theta=\mathscr{C}} \\ &= (K_0 + \langle u, y\rangle)\,E + \mathscr{H}(X_{K_0}) + \underbrace{A^* u}_{\in\ker\theta=\mathscr{C}} \\ &= \underbrace{X_{K_0}}_{\text{drift contact vect. field}} + \underbrace{\underbrace{\langle u, y\rangle\,E}_{\in\ker d\theta} + \underbrace{A^* u}_{\in\ker\theta=\mathscr{C}}}_{\text{control vect. field}} \end{aligned} \tag{23}$$

Variational contact systems as explicit nonlinear system (1)

The output variable y satisfies

$$\frac{d}{dt} y = A \circ d\theta \left(X \left(\tilde{x}, u, y \right) \right) \tag{24}$$

But

$$\begin{aligned} d\theta \left(X \left(\tilde{x}, u, y \right) \right) &= i_{X(\tilde{x}, u, y)} d\theta \\ &= i_{X_{K_0}} d\theta + \langle u, y \rangle \underbrace{i_E d\theta}_{=0} + d\theta \left(A^* u \right) \\ &= -\left(dK_0 - \left(i_E dK_0 \right) \theta \right) + d\theta \left(A^* u \right) \end{aligned}$$

hence the dynamics of the output becomes

$$\frac{d}{dt} y = -A(dK_0) + (A \circ d\theta \circ A^*) u$$

Relation with input-output contact systems

The conservative contact input-output system with internal contact Hamiltonian $K_0(\tilde{x})$ and control contact Hamiltonians $-K_i(\tilde{x})$ is a variational control contact system with internal contact Hamiltonian $K_0(\tilde{x})$ and bundle map $A : T^*\mathscr{M} \to \mathbb{R}^n \times \mathscr{M}$ defined by

$$A(\lambda) = (A_i(\lambda))_{i=1,\dots,m} = (\langle \lambda, \mathscr{H}(X_{K_i}) \rangle)_{i=1,\dots,m} \tag{25}$$

Feedback invariance of control contact systems

Feedback invariance of control contact systems

Objectives

We would like to investigate the abstract problem about state-feedback of single input control contact systems, affine in the input :

under which conditions is the closed-loop system again a contact system ?

Based on

1. H. Ramırez Estay , B. Maschke and D. Sbarbaro, *Feedback equivalence of input-output contact systems*, **Systems and Control Letters**, Volume 62, Issue 6, pp. 475-481, June 2013
2. H. Ramirez, B. Maschke and Daniel Sbarbaro, *Partial stabilization of input-output contact systems on a Legendre submanifold* , **IEEE Transaction on Automatic Control**, Vol. 62, n°3, pp. 1431 - 1437, March 2017

Control contact systems

Control contact systems are defined by contact Hamiltonians which depend not only on the state variables $\tilde{x}$ but also on a time dependent input function $u(t) \in L_1^{\mathrm{loc}}(\mathbb{R}_+)$ as control Hamiltonian systems.

Definition

Control contact systems affine in the input are defined by $\frac{d}{dt}\tilde{x} = X$

$$X = X_{K_0} + X_{K_c} u \tag{26}$$

where $K_0 \in C^\infty(\mathscr{M})$ is the *internal contact Hamiltonian* and $K_c \in C^\infty(\mathscr{M})$ is the *interaction (or control) contact Hamiltonian* and where X_{K_0} and X_{K_c} are contact vector fields with respect to the canonical contact form θ.

Structure preserving feedback

Structure preserving feedback

State feedback leaving the contact form invariant

When does a state feedback $u = \alpha(\tilde{x})$, with $\alpha \in C^\infty(\mathscr{M})$, generates a closed-loop vector field $X = X_{K_0} + X_{K_c}\alpha$ that is again a contact vector field with respect to the contact form θ ?

Theorem

Consider the controlled contact system with the condition that K_c vanishes on a submanifold of measure 0 (that is, is fully actuated) and the feedback $u = \alpha(\tilde{x})$ being a smooth function of the state variables. The closed loop vector field X is a contact vector field with respect to the canonical contact form θ if and only if $\alpha(\tilde{x}) = \alpha_{cte}$ is constant.

Proof

Using Cartan's formula: $L_X \cdot = i_X d \cdot + d i_X \cdot$., one obtains:

$$L_X \theta = L_{X_{K_0} + \alpha X_{K_c}} \theta = (\rho_0 + \alpha \rho_c) \theta + K_c d\alpha \qquad (27)$$

where $\rho_0 = i_E dK_0$ and $\rho_c = i_E dK_c$.
This is equivalent to the existence of a function $\phi \in C^\infty(\mathscr{M})$ such that: $K_c d\alpha = \phi \theta$.
In canonical coordinates, we may write

$$K_c \left(\frac{\partial \alpha}{\partial x^0} dx^0 + \sum_{k=1}^{n} \frac{\partial \alpha}{\partial x^k} dx^k + \sum_{k=1}^{n} \frac{\partial \alpha}{\partial p_k} dp_k \right) = \phi dx^0 - \sum_{k=1}^{n} p_k dx^k,$$

which by smoothness of the functions and as K_c vanishes on a submanifold of measure 0 leads to $\frac{\partial \alpha}{\partial x^k} = -\frac{\partial \alpha}{\partial x^0} p_k$ and $\frac{\partial \alpha}{\partial p_k} = 0$, which implies that α is constant.

Feedback equivalence with a contact vector field with respect to a different contact form

When does a state feedback $u = \alpha(\tilde{x})$ define the closed-loop contact vector field $X = X_{K_0} + X_{K_c}\alpha$, as a contact vector field with respect to a new contact form θ_d ?

Therefore we consider the equivalent condition of the existence of a function $\rho_d \in C^\infty(\mathscr{M})$ such that $L_X\theta_d = \rho_d\theta_d$.

The problem is formulated : under which conditions there exist a contact form θ_d, a function $\rho_d \in C^\infty(\mathscr{M})$ and a feedback $u = \alpha \in C^\infty(\mathscr{M})$ such that the following matching equation is satisfied

$$\rho_d\theta_d = L_{X_{K_0}}\theta_d + \alpha L_{X_{K_c}}\theta_d + (i_{X_{K_C}}\theta_d)d\alpha. \qquad (28)$$

Matching equation for strict contact vector fields

Matching equation for strict contact vector fields

Matching equation for strict contact vector fields

We assume in the sequel that the internal and control contact Hamiltonian and the closed-loop contact Hamiltonian do not depend on the coordinate x_0 hence $\rho_d = \rho_0 = \rho_c = 0$.

This is not a restrictive assumption since for contact systems arising from the modelling of physical systems, the contact Hamiltonian indeed do not depend on the x_0 coordinate representing the energy (or more generally a thermodynamic potential) .

Under this assumption the matching equation (28) is reduced to a relation on the feedback α and the closed-loop contact structure θ_d

$$L_{X_{K_0}} \theta_d + \alpha L_{X_{K_c}} \theta_d + (i_{X_{K_C}} \theta_d) d\alpha = 0. \tag{29}$$

Matching to a contact form obtained by adding an exact form

We shall restrict the closed-loop contact form θ_d defined as

$$\theta_d = \theta + dF, \tag{30}$$

with $F \in C^\infty(\mathscr{M})$ satisfying $i_E dF = 0$.

Note that the condition $i_E dF = 0$ is equivalent in canonical coordinates to assume that the function F depends only on (x, p) and not on x_0.

Theorem

The 1-form defined by (30) is a contact form.

Proof (1)

Recall that θ_d is a contact form if it is a Pfaffian form of class $2n+1$, satisfying ,

$$\theta_d \wedge (d\theta_d)^n \neq 0, \tag{31}$$

$$\theta_d \wedge (d\theta_d)^{n+1} = 0. \tag{32}$$

Consider first the inequality (31). Note that using $d^2 F = 0$ one has that

$$\begin{aligned} \theta_d \wedge (d\theta_d)^n &= (\theta + dF) \wedge (d(\theta + dF))^n \\ &= (\theta + dF) \wedge (d\theta)^n \end{aligned}$$

Proof (2)

Now proceed by contradiction and assume that $\theta_d \wedge (d\theta_d)^n = 0$. Then, using the fact that i_E is a $\wedge$ antiderivation and the properties of the Reeb vector field:

$$
\begin{aligned}
& i_E \left[\theta_d \wedge (d\theta_d)^n\right] \\
& \quad = i_E \left[(\theta + dF) \wedge (d\theta)^n\right] \\
& \quad = i_E(\theta + dF) \wedge (d\theta)^n + (-1)(\theta + dF) \wedge i_E\left((d\theta)^n\right) \\
& \quad = (1 + i_E dF) \wedge (d\theta)^n
\end{aligned}
$$

and $i_E dF = 0$, implies that $(d\theta)^n = 0$ which is contradicting the fact that θ is of class $2n+1$.

Proof (3) and interpretation of the closed-loop contact structure

To check $\theta_d \wedge (d\theta_d)^{n+1} = 0$ notice that $(d\theta)^{n+1}$ is full rank, hence $dF \wedge (d\theta)^{n+1} = 0$ no matter the choice of F and

$$\begin{aligned} \theta_d \wedge (d\theta_d)^{n+1} &= \theta \wedge (d\theta)^{n+1} + dF \wedge (d\theta)^{n+1} \\ &= \theta \wedge (d\theta)^{n+1} = 0 \end{aligned}$$

The closed-loop contact form is thus given by

$$\begin{aligned} \theta_d = \theta + dF &= \left(dx_0 - \sum_{i=1}^{n} p_i dx_i \right) + dF, \\ &= d(x_0 + F) - \sum_{i=1}^{n} p_i dx_i . \end{aligned}$$

Matching equation in terms of feedback and added form

The matching equation may finally be rewritten as the following matching equation in the feedback α and the function F

$$d(X(F)) + K_c d\alpha = 0. \tag{33}$$

Taking the exterior derivative of (33) we get $dK_c \wedge d\alpha = 0$ which leads to consider $\alpha = \varphi \circ K_c$.

The closed-loop vector field$X$ may be defined as a contact vector field with respect to the contact form θ_d

$$X = X_{K_0} + \alpha X_{K_c} = \hat{X}_K \tag{34}$$

and generated by $K = K_0 + X_{K_0}(F) + \alpha(K_c + X_{K_c}(F))$.

Decoupling the matching equation

Theorem

Define $K_0, K_c, F \in \mathscr{C}^\infty(\mathscr{M})$, *satisfying* $i_E. = 0$, *with closed-loop contact form* $\theta_d = \theta + dF$ *and state-feedback*

$$\alpha = \varphi \circ K_c$$

where $\varphi \in C^\infty(\mathbb{R})$, *then*
$X = X_{K_0} + \alpha X_{Kc}$ *is contact vector field with respect to* θ_d *iff*

$$X_{K_0}(F) + (\varphi \circ K_c)[K_c + X_{K_c}(F)] - \Phi \circ K_c = c_F$$

with $\Phi(\lambda) = \int_0^\lambda \varphi(\lambda)\, d\chi$.
Furthermore the closed-loop Hamiltonian is $K = K_0 + \Phi \circ K_c$.

Some remarks on control synthesis

We have shown that the control is defined by a function $\varphi \in C^\infty(\mathbb{R})$ as : $\alpha = \varphi \circ K_c$.
Once the choice of this function φ is made one has still to consider the matching equation n F:

$$X_{K_0}(F) + (\varphi \circ K_c)[K_c + X_{K_c}(F)] - \Phi \circ K_c = c_F$$

which is written in canonical coordinates :

$$\begin{bmatrix} \frac{\partial F}{\partial x} \\ \frac{\partial F}{\partial p} \end{bmatrix}^\top \begin{bmatrix} -\frac{\partial K_0}{\partial p} - (\varphi \circ K_c)\frac{\partial K_c}{\partial p} \\ \frac{\partial K_0}{\partial x} + (\varphi \circ K_c)\frac{\partial K_c}{\partial x} \end{bmatrix} + (\varphi \circ K_c)K_c - \Phi \circ K_c = 0. \qquad (35)$$

and is a quasi-linear PDE in F .

Stabilizing structure preserving feedback control

Stabilizing structure preserving feedback control

On the stability of contact vector fields

On the stability of contact vector fields

Equilibria of a contact system: reminder

Theorem

Consider a contact manifold $(\mathscr{M}, \theta)$ and a strict contact vector field X_K generated by the contact Hamiltonian $K(\tilde{x}) \in C^\infty(\mathscr{M})$ (satifying $i_E dK = 0$). and the contact system defined by

$$\frac{d}{dt}\tilde{x} = X_K(\tilde{x}) \tag{36}$$

then a point $\tilde{x}^* \in \mathscr{M}$ is an equilibrium point of the contact system if and only if it satisfies

$$K(\tilde{x}^*) = 0$$

$$dK(\tilde{x}^*) = 0$$

The submanifold of the zeros of the contact Hamiltonian $S = K^{-1}(0)$

In the sequel we shall consider the set

$$S = K^{-1}(0)$$

and assume some regularity of Hamiltonian $K(\tilde{x})$.

Assumption

The set $S = K^{-1}(0)$ is a differentiable manifold of constant dimension $2n$.

Note that the set S contains:

- all equilibrium points
- the Legendre submanifold $\mathscr{L}_U$ defining the thermodynamic properties for a *conservative* system

Invariance of the submanifold $S = K^{-1}(0)$

Proposition

The contact vector field X_K with contact Hamiltonian K being an invariant of the Reeb vector field, leaves any submanifold $K^{-1}(c)$, $c \in \mathbb{R}$ invariant.

Using the Jacobi bracket $[\,,]_\theta$ induced by θ, one has

$$L_{X_K} K = i_{X_K} dK = \underbrace{[K, K]_\theta}_{=0} + K \underbrace{i_E dK}_{=0} = 0$$

as the Jacobi bracket is anti-symmetric and the contact Hamiltonian is an invariant of the Reeb vector field, that is: $i_E dK = 0$.

About the stability of equilibria points relatively to $S = K^{-1}(0)$

In the sequel we shall analyze
the stability relatively to the invariant manifold $S = K^{-1}(0)$,
i.e. the stability of the restriction $\bar{X}_K = X_K|_S$ of the strict contact vector field on the submanifold $S = K^{-1}(0)$

Theorem

Let $\tilde{x}^* \in S$ be an hyperbolic critical point of the restriction $\bar{X}_K$ of the strict contact vector field on the submanifold $S = K^{-1}(0)$. The stable manifold $S^+(\{\tilde{x}^*\})$ and the unstable manifold $S^-(\{\tilde{x}^*\})$ are Legendre submanifolds of $(\mathscr{M}, \theta)$.

Proof (1)

By assumption, the vector field $\bar{X}_K$ is complete and denote by φ_t its integral flow.
As it is the restriction of the contact vector field X_K, one has

$$\theta(s)\left(\bar{X}_K(s)\right) = \theta(\varphi_t(s))\left(\varphi_t(s)_* \bar{X}_K(s)\right)$$
$$\forall s \in S^+(\{\tilde{x}^*\}),\ t \in \mathbb{R}_+.$$

As the vector field $\bar{X}_K$ generates an orbit converging to the equilibrium point $\tilde{x}^*$,

$$\lim_{t \to +\infty} \varphi_t(s)_* \bar{X}_K(s) = 0$$

hence

$$\theta(s)\left(\bar{X}_K(s)\right) = 0 \quad \forall s \in S^+(\{\tilde{x}^*\}),\ \bar{X}_K \in T_s S^+(\{\tilde{x}^*\}) \qquad (37)$$

Proof (2)

As a consequence, the stable manifold by $S^+(\{\tilde{x}^*\})$ is an integral manifold of θ of dimension less or equal than n.

It may be shown with similar arguments (but reversing the time limit) that the unstable manifold $S^-(\{\tilde{x}^*\})$ is also an integral manifold of θ and has dimension less or equal than n.

As the equilibrium point is assumed to be hyperbolic, the stable and unstable submanifolds have complementary dimensions in $S = K^{-1}(0)$ which by assumption has dimension $2n$.
Hence both the stable and unstable submanifolds have the maximal dimension n and are Legendre submanifolds.

Partial stabilization on a Legendre submanifold

Partial stabilization on a Legendre submanifold

Control objective: stabilization

As a consequence, any state-feedback control

$$\alpha = \varphi \circ K_c$$

which preserves the contact strucure in the sense that the closed-loop system is again a conservative contact system defined by the strict contact vector field

$$X = X_{K_0} + \alpha X_{Kc}$$

is contact vector field with respect to $\theta_d = \theta + dF$ **may at most stabilize the input-output contact system on a Legendre submanifold** being the stable manifold by $S^+(\{\tilde{x}^*\})$ of X.

Control objective: shaping the equilibrium and non-equilibrium properties

Hence we shall state-feedback control

$$\alpha = \varphi \circ K_c$$

such that the closed-loop system is again a conservative contact system defined by the strict contact vector field with respect to the contact form θ_d

$$X = X_{K_0} + \alpha X_{K_c} = \hat{X}_K$$

1. generated by $K_d = K_0 + X_{K_0}(F) + \alpha(K_c + X_{K_c}(F))$: non-equilibrium
2. leaving invariant the Legendre submanifold $\mathfrak{L}_{Ud}$ generated by the closed-loop generating function U_d: equilibrium

2 cells with thermostat as a port contact system

- Thermodynamic phase space has the coordinates: energy x^0, entropies $x^i \in \mathcal{N} = \mathbb{R}^2$, temperature $p_i \in T_S^*\mathcal{N} \approx \mathbb{R}^2$
- with contact form $\theta = dx^0 - p_i dx^i$
- a Legendre submanifold $\mathcal{L} \ni \left(U, S^i, T_i\right)$ generated by the internal energy $U(S)$
- the internal contact Hamiltonian:

$$K_0 = -Rp^\top JT - (T_2 - p_2)\lambda_e \frac{p_2}{T_2}, \quad K_c = e^{-\lambda_e\left(\frac{p_2}{T_2} - 1\right)} - 1 \qquad (38)$$

- the control Hamiltonian:

$$K_c(x,p) = e^{-\lambda_e\left(\frac{p_2}{T_2} - 1\right)} - 1 \qquad (39)$$

2 cells with thermostat: control

A structure preserving output feedback $\alpha = \Phi'(y)$ is:

$$\alpha(x_2, p_2) = \Phi' \circ K_c(x_2, p_2) = \beta\left(\lambda_e \frac{p_2 - T_2}{T_2}\right), \ \beta \in C^\infty(\mathbb{R})$$

The actual state feedback is restricted to the closed-loop Legendre submanifold $\mathscr{L}_{U_d}$ defined with respect to the generating function $U_d(x)$:

$$u(x_1, x_2) = \beta\left(\underbrace{\lambda_e \frac{\frac{\partial U_d}{\partial x_2}(x_1, x_2) - T_2(x_2)}{T_2(x_2)}}_{\text{control entropy flux}}\right)$$

which may be interpreted as a nonlinear function of a "control" entropy flux into the compartment 2 induced by a (thermostat) control temperature $\frac{\partial U_d}{\partial x_2}(x_1, x_2)$ defined by the closed-loop Legendre submanifold $\mathfrak{L}_{Ud}$.

Conclusion

Conclusion

Control contact systems on Thermodynamic Phase Space

Implicit formulation of balance equations including energy and entropy balance. Alternative formulations

- energy formulation $dU = TdS + (-P)dV + \mu dN$
  - D. Eberard, B.M. Maschke, and A.J. van der Schaft. *An extension of pseudo-Hamiltonian systems to the thermodynamic space : towards a geometry of non-equilibrium thermodynamics*. **Reports on Mathematical Physics**, 60(2) :175–198, 2007
  - H. Ramırez Estay , B. Maschke and D. Sbarbaro, *Irreversible port-Hamiltonian systems : A general formulation of irreversible processes with application to the CSTR*, **Chemical Engineering Science**, Volume 89, pp. 223-234 15 February 2013
- entropy formulation $dS = \frac{1}{T}dU + \frac{P}{T}dV - \frac{\mu^t}{T}dn$
  - Favache, D. Dochain and B. Maschke, *An entropy-based formulation of irreversible processes based on contact structures*, **Chemical Engineering Science**, vol. 65, pp. 5204-5216, 2010

Conservative control contact sytems describe quasi-reversible processes.

Structure preserving control

The result about the state feedback of control contact systems :

- qualifies the control contact Hamiltonian K_c as natural output
- imposes a closed-loop contact structure different from open-loop one

H. Ramırez Estay , B. Maschke and D. Sbarbaro, Feedback equivalence of input-output contact systems, **Systems and Control Letters**, Volume 62, Issue 6, pp. 475-481, June 2013

H. Ramirez, B. Maschke and Daniel Sbarbaro, Partial stabilization of input-output contact systems on a Legendre submanifold , **IEEE Transaction on Automatic Control**, Vol. 62, n°3, pp. 1431 - 1437, March 2017

Structure preserving control

Remains to consider the control design in order to :

- shape the losed-loop contact Hamiltonian function/the closed-loop Legendre submanifold
- apply to chemical reactor

Generalize to:

- more general closed-loop contact forms than $\theta_d = \theta + dF(q, p)$
- closed-loop contact systems which do not leave invariant any Legendre submanifold and lead to dynamic feedback.