Port Maps for Irreversible Interface Relations

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Introduction

Port maps arizing from Poisson brackets Irreversible Hamiltonian systems Irreversible Port Hamiltonian Systems Conclusion



Introduction

Bernhard Maschke Port Maps for Irreversible Interface Relations

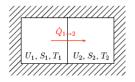
Motivation : Port maps for Irreversible Port Hamiltonian Systems

- Irreversible Hamiltonian Sytems :
 - geometry represents the topology, the energy fluxes within and with its environment
 - represents the reversible and irreversible phenomena
- Port conjugated output not defined for Irreversible Port Hamiltonian Systems requires to distinguish
 - interface which are subject to irreversible phenomena such as Fourier's law or not
 - for such interface make appear the entropy creation at the interface and deduce the port maps

Introduction

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Heat exchanger : failure of Hamiltonian framework



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 : $\dot{Q}_{1\rightarrow 2} = -T_1 \frac{dS_i}{dt} = T_2 \frac{dS_2}{dt}$ lead to the entropy balance equations

$$\frac{d}{dt} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \begin{pmatrix} -\frac{\dot{Q}_{1\to 2}}{T_1} \\ \frac{\dot{Q}_{1\to 2}}{T_2} \end{pmatrix} = \lambda \left(\frac{1}{T_2} - \frac{1}{T_1}\right) \begin{pmatrix} -T_2 \\ T_1 \end{pmatrix}$$

Heat exchanger : failure of Hamiltonian framework Heat conduction process : pseudo-Hamiltonian formulation

The Hamiltonian-like formulation :

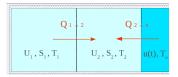
$$\frac{d}{dt} \begin{pmatrix} S_1 \\ S_2 \end{pmatrix} = \underbrace{\lambda \left(\frac{1}{T_2} - \frac{1}{T_1}\right) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}}_{J(T)} \begin{pmatrix} T_1 \\ T_2 \end{pmatrix}$$

with $T_i = \frac{\partial (U_1 + U_2)}{\partial S_i}(S) = \frac{\partial U_i}{\partial S_i}(S_i)$.

- J(T) is skew-symmetric but depend on the temperature and not the entropy.
- 3 the map from the gradient of the total energy $\frac{\partial(U_1+U_2)}{\partial S}$ to the generalized velocities is not linear!

Heat exchanger with thermostat

Two systems 1 and 2 interact through a heat conducting conducting wall and system 2 interacts with a thermostat at temperature T_e : input map affine in the control ! Port conjugated output ?



The entropy balance equations

$$\begin{bmatrix} \dot{S}_1 \\ \dot{S}_2 \end{bmatrix} = \lambda \begin{bmatrix} \frac{T_2(S_2)}{T_1(S_1)} - 1 \\ \frac{T_1(S_1)}{T_2(S_2)} - 1 \end{bmatrix} + \lambda_e \begin{bmatrix} 0 \\ \frac{T_e(t)}{T_2(S_2)} - 1 \end{bmatrix}$$

where S_1 and S_2 are the entropies of subsystem 1 and 2, $T_e(t)$ a time dependent external heat source and $\lambda > 0$ and $\lambda_e > 0$ denotes Fourier's heat conduction coefficients of the internal wall and the external wall.

Complete the Irrreversible Port Hamiltonian Systems

Irreversible Port Hamiltonian Systems (IPHS) is the nonlinear control system

$$\frac{dx}{dt} = m\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right) J \frac{\partial H}{\partial x}(x) + W\left(x, \frac{\partial H}{\partial x}\right) + g\left(x, \frac{\partial H}{\partial x}\right) u, \quad (1)$$

generated by two function H(x) and S(x) !

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

H. Ramırez Estay , B. Maschke and D. Sbarbaro, Irreversible port Hamiltonian systems, European Journal of Control, Special issue "Lagrangian and Hamiltonian methods for non-linear control", A. Macchelli and C . Secchi eds., , Volume 19, n° 6, pp.513-520, 2013

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Port Hamiltonian systems: conjugated port maps

Port Hamiltonian systems: conjugated port maps

Port Hamiltonian systems

Port Hamiltonian Systems are non-linear control systems

$$\begin{pmatrix} \frac{dx}{dt} \\ -y \end{pmatrix} = \begin{pmatrix} J(x) & g(x) \\ -g(x)^{\top} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial x} \\ u \end{pmatrix}$$
(2)

defined by

- **(**) the state vector $x \in \mathbb{R}^n = \mathscr{X}$,
- ② the Hamiltonian function H(x) : $\mathscr{C}^{\infty}(\mathbb{R}^n) \to \mathbb{R}$
- **③** the skew-symmetric structure matrix $J(x) \in \mathbb{R}^n \times \mathbb{R}^n$
- the input matrix g(x)

The anti-adjoint maps defined by g(x) and $-g^{\top}(x)$ define pairs of conjugated port variables (u, y) and the balance equation

$$\frac{dH}{dt} = y^\top u$$

Port Hamiltonian systems

The map $T^*\mathscr{X} \times U \to T\mathscr{X} \times Y$ defined by

$$\begin{pmatrix} J(x) & g(x) \\ -g(x)^{\top} & 0 \end{pmatrix}$$
(3)

extends the (pseudo-)Poisson bracket associated with the skew-symmetric matrix J(x) and may be seen as arizing from the (pseudo-)Hamiltonian system

$$\begin{pmatrix} \frac{dx}{dt} \\ \frac{d\xi}{dt} \end{pmatrix} = \begin{pmatrix} J(x) & g(x) \\ -g(x)^{\top} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial x}(x) \\ \frac{\partial H_{u}}{\partial \xi}(\xi) \end{pmatrix}$$

with $\xi(t) \in \mathbb{R}^m$ is the state variable of the environment and Hamiltonian function being linear in the input u:

$$\bar{H}_u(\xi) = u^\top \xi \tag{4}$$

and projected parallel to the environment's state.

Irreversible Hamiltonian systems Canonical example : heat exchanger

Irreversible Port Hamiltonian systems

Irreversible Port Hamiltonian systems

Irreversible Hamiltonian systems Canonical example : heat exchanger

A class of quasi-Hamiltonian systems : irreversible Hamiltonian systems

Irreversible HS are defined by the following dynamic equation

$$\dot{x} = \gamma\left(x, \frac{\partial U}{\partial x}\right) \underbrace{\frac{\partial S}{\partial x}(x)^{T} J \frac{\partial U}{\partial x}(x)}_{=\{S, U\}_{J}} J \frac{\partial U}{\partial x}(x)$$

with

- the state vector $x \in \mathbb{R}^n$, the energy function $U(x) : \mathscr{C}^{\infty}(\mathbb{R}^n) \to \mathbb{R}$ and the entropy function $S(x) : \mathscr{C}^{\infty}(\mathbb{R}^n) \to \mathbb{R}$.
- 2 the constant skew-symmetric structure matrix $J \in \mathbb{R}^n \times \mathbb{R}^n$
- **3** a positive definite function: $\gamma(x, \frac{\partial U}{\partial x}) = \hat{\gamma}(x) : \mathscr{C}^{\infty}(\mathbb{R}^n) \to \mathbb{R}^*_+$.

Irreversible Hamiltonian systems Canonical example : heat exchanger

Irreversible Hamiltonian systems : energy and entropy balance equations

The conservation equation of the internal energy,

$$\frac{dU}{dt} = 0, \tag{5}$$

follows from the skew-symmetry of the structure matrix J.

The irreversible entropy production

$$\frac{dS}{dt} = \gamma\left(x, \frac{\partial U}{\partial x}\right) \{S, U\}_J^2 \ge 0$$

Irreversible Port Hamiltonian arize naturally for heat exchangers, Chemical reactors, etc..:

- the bracket $\{S, H\}_J$ is the thermodynamic force
- the function $\gamma\left(x,\frac{\partial U}{\partial x}\right)$ the irreversible phenomenon relation

Irreversible Hamiltonian systems Canonical example : heat exchanger

Canonical example : the heat exchanger

Canonical example: the heat exchanger

Irreversible Hamiltonian systems Canonical example : heat exchanger

Heat conduction : irreversible Hamiltonian system

$$\frac{d}{dt}\begin{pmatrix}S_1\\S_2\end{pmatrix} = \lambda\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\begin{bmatrix}0 & -1\\1 & 0\end{bmatrix}\begin{bmatrix}T_1\\T_2\end{bmatrix} \\ = \underbrace{\lambda}_{=\gamma}\underbrace{(T_1 - T_2)}_{=\{S, U\}_J}\begin{bmatrix}0 & -1\\1 & 0\end{bmatrix}\underbrace{(T_1\\T_2]}_{dU(S)}$$

with :

• internal energy U, co-energy variables : $\frac{\partial U}{\partial S_i} = T_i(S_i)$ • entropy function : $\mathscr{S} = S_1 + S_2$ and $\frac{\partial \mathscr{S}}{\partial x}^{\top} J \frac{\partial U}{\partial x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}^{\top} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} = T_1 - T_2$: driving force • positive function : $\gamma \left(\frac{\partial U}{\partial S}\right) = \frac{\lambda}{T_1 T_2} > 0$ as $T_1 > 0$ and $T_2 > 0$: Fourier's law

Irreversible Hamiltonian systems Canonical example : heat exchanger

Heat exchanger : internal energy and entropy balance equations Energy and entropy balance equations

Conservation of the total internal energy due to the skew-symmetry of J(T):

$$\frac{d}{dt}(U_1+U_2)=(T_1, T_2)\lambda\left(\frac{1}{T_2}-\frac{1}{T_1}\right)\begin{pmatrix}0 & -1\\1 & 0\end{pmatrix}\begin{pmatrix}T_1\\T_2\end{pmatrix}=0$$

Increase of the total entropy due to the non-linear map :

$$\frac{d}{dt}(S_1+S_2)=(1,1)\lambda\left(\frac{1}{T_2}-\frac{1}{T_1}\right)\begin{pmatrix}0&-1\\1&0\end{pmatrix}\begin{pmatrix}T_1\\T_2\end{pmatrix}=\lambda\frac{(T_1-T_2)^2}{T_1T_2}\geq 0$$

Irreversible Hamiltonian systems Canonical example : heat exchanger

Reversible-Irreversible Hamiltonian systems

$$\frac{dx}{dt} = \left[\underbrace{\underbrace{J_0(x)}_{\text{reversible}} + \underbrace{\gamma\left(x, \frac{\partial H}{\partial x}\right)\left\{S, H\right\}_J J}_{\text{irreversible coupling}}\right] \frac{\partial U}{\partial x}(x)$$
(6)

where

(i) $J_0(x)$ and J the structure matrix of a Poisson bracket (ii) $\gamma(x, \frac{\partial H}{\partial x}) > 0$ (iii) the entropy function S(x) a Casimir function of the Poisson

structure matrix $J_0(x)$

Satisfies the two balance equations:

- conservation equation of the internal energy, $\frac{dU}{dt} = 0$,
- entropy balance equation with irreversible entropy production $\frac{dS}{dt} = \gamma\left(x, \frac{\partial U}{\partial x}\right) \{S, U\}_{J}^{2} \ge 0$

Definition Example : Heat exchanger with thermostat

Irreversible Port Hamiltonian systems

Irreversible Port Hamiltonian systems

Definition Example : Heat exchanger with thermostat

Port map arizing from a IHS: extended system

Consider

- state variablex $(t) \in \mathbb{R}^n$
- environment state $\xi\left(t
 ight)\in\mathbb{R}^{m}$
- constant structure matrix defined by $g \in \mathbb{R}^{n imes m}$

$$J_{\text{port}} = \left(\begin{array}{cc} 0 & g \\ -g^{\top} & 0 \end{array}\right)$$

energy function

$$H_{\text{tot}}(x,\xi) = H(x) + u^{\top}\xi$$
, $u \in \mathbb{R}^m$

entropy function

$$S_{ ext{tot}}(x,\xi) = S(x) + au^{ op} \xi \ , \quad au \in \mathbb{R}^m$$

Definition Example : Heat exchanger with thermostat

Port map arizing from a IHS: Irreversible Port Hamiltonian System

$$\begin{pmatrix} \frac{dx}{dt} \\ -y \end{pmatrix} = \gamma_{\text{port}} \left(x, \frac{\partial H}{\partial x}, u \right) \{S_{\text{tot}}, H_{\text{tot}}\}_{J_{\text{port}}} \underbrace{J_{\text{port}} \left(\begin{array}{c} \frac{\partial H}{\partial x} \\ u \end{array} \right)}_{= \left(\begin{array}{c} g u \\ -g^{\top} \frac{\partial H}{\partial x} \end{array} \right)}$$

where $\{S_{\text{tot}}, H_{\text{tot}}\}_{J_{\text{port}}} = \left[\left(g^{\top} \frac{\partial S}{\partial x} \right)^{\top} u - \tau^{\top} \left(g^{\top} \frac{\partial H}{\partial x} \right) \right]$
• $u = \frac{\partial H_{\text{tot}}(x,\xi)}{\partial \xi}$ and $\tau = \frac{\partial S_{\text{tot}}(x,\xi)}{\partial \xi}$
• $\gamma_{\text{port}} \left(x, \frac{\partial H}{\partial x}, u \right)$ is a strictly positive function.

Definition Example : Heat exchanger with thermostat

Irreversible Port Hamiltonian systems

An Irreversible Port Hamiltonian system (IPHS)

$$\frac{dx}{dt} = \gamma\left(x, \frac{\partial H}{\partial x}\right) \{S, H\}_{J} J \frac{\partial H}{\partial x}(x)$$

$$+ \gamma_{\text{port}}\left(x, \frac{\partial H}{\partial x}, u\right) \left[\left(g^{\top} \frac{\partial S}{\partial x}\right)^{\top} u - \tau^{\top} \left(g^{\top} \frac{\partial H}{\partial x}\right) \right] g u \quad (8)$$

$$y = \gamma_{\text{port}}\left(x, \frac{\partial H}{\partial x}, u\right) \left[\left(g^{\top} \frac{\partial S}{\partial x}\right)^{\top} u - \tau^{\top} \left(g^{\top} \frac{\partial H}{\partial x}\right) \right] g^{\top} \frac{\partial H}{\partial x} (9)$$

(i) a real function $\gamma_{\text{port}}\left(x, \frac{\partial H}{\partial x}, u\right)$, strictly positive function (iv) the input vctor field $g \in \mathbb{R}^{n \times m}$ and the vector $\tau \in \mathbb{R}^m$ associated with the ports of the system.

Definition Example : Heat exchanger with thermostat

Energy and entropy balance equations

The energy balance equation

$$\frac{dH}{dt} - y^{\top}u = 0$$

where $y^{\top}u$ is the power flowing into the system The entropy balance equation

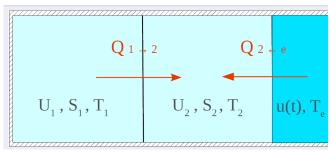
$$\begin{aligned} \frac{dS}{dt} - \tau^{\top} y &= \gamma \left(x, \frac{\partial U}{\partial x} \right) \{ S, U \}_{J}^{2} \\ &+ \gamma_{\text{port}} \left(x, \frac{\partial H}{\partial x}, u \right) \left[\left(g^{\top} \frac{\partial S}{\partial x} \right)^{\top} u - \tau^{\top} \left(g^{\top} \frac{\partial H}{\partial x} \right) \right]^{2} \geq 0 \end{aligned}$$

where the term $\tau^{\top} y$ corresponds to the entropy flowing out the environment (to the system).

Definition Example : Heat exchanger with thermostat

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 .



The entropy balance equations

$$\begin{bmatrix} \dot{S}_1\\ \dot{S}_2 \end{bmatrix} = \lambda \begin{bmatrix} \frac{T_2(S_2)}{T_1(S_1)} - 1\\ T_1(S_1) \end{bmatrix} + \lambda_e \begin{bmatrix} 0\\ \frac{T_e(t)}{T_e(t)} - 1 \end{bmatrix}$$
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Definition Example : Heat exchanger with thermostat

Heat conduction : irreversible Hamiltonian system

$$\frac{d}{dt} \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} = \frac{\lambda}{\underbrace{T_1 T_2}} \underbrace{(T_1 - T_2)}_{=\{S, U\}_J} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \underbrace{\begin{bmatrix} T_1 \\ T_2 \end{bmatrix}}_{dU(S)} + \underbrace{\frac{\lambda_e}{T_2 u}}_{=\gamma_{\text{port}}(T_2, u)} \underbrace{(u - T_2)}_{=g} \underbrace{\begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{=g} u$$

and output being the entropy flux leaving the environment (with respect to the temperature $u = T_e$ of the environment).

$$y = \frac{\lambda_e}{uT_2} \left[(u - T_2) \right] \left[\begin{array}{c} 0 & 1 \end{array} \right] \left[\begin{array}{c} T_1 \\ T_2 \end{array} \right] = \frac{\lambda_e \left(u - T_2 \right)}{u}$$

with :

- the port map defined by the vector $g=\left(egin{array}{c} 0\\ 1\end{array}
 ight)$
- input the temperature $u=T_e$ of the environment and au=1
- function $\gamma_{\text{port}}(T_2, u) = \frac{\lambda_e}{uT_2}$ (which is well-defined for u > 0)



Conclusion

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Conclusion

- We have discussed the Port maps defining the pairs of conjugated port variables:
 - for reversible Port Hamiltonian Systems as a projection of a coupled system with a state space representation of the environment with linear Hamiltonian function
 - for Irreversible Port Hamiltonian Systemswe have suhh-ggested an extension by introducing a second input related to the definition of an entropy function for the environment and derived the associated output port variable.
- Current and ongoing work:
 - develop time discretization schemes preserving the energy and entropy balance : with David Martin de Diego and Laurent Lefèvre
 - develop optimal control using the energy and entropy as cost functions: Timm Faulwasser, Friedrich Philipp, Manuel