



From reversible to irreversible thermodynamic formulations : modelling

Yann Le Gorrec¹ and Hector Ramirez

¹ SupMicroTech Besançon FEMTO-ST
Joint work with Bernhard Maschke and Luis Mora.

Funded by the European Project ModConflex





1. Context, motivation
2. A simple but instructive example
3. Infinite dimensional irreversible port Hamiltonian systems (IPHS)
4. Conclusions



Context, motivation

- In many cutting-edge engineering applications, for example within the field of soft or micro-nano robotics, process control, material sciences, energy production etc ... **temperature plays a central role** and needs to be explicitly taken into account.

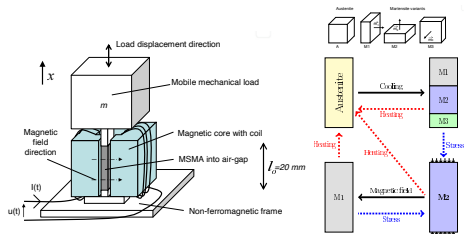


Figure: MSMA actuator.

Cf. Hector's talk on IPHS for finite dimensional systems.

Context, motivation

- Some examples of Distributed Parameter Systems for which the thermal domain plays a central role

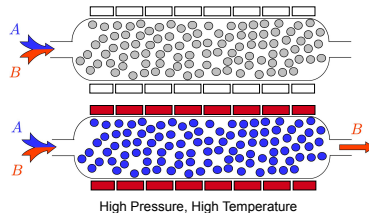


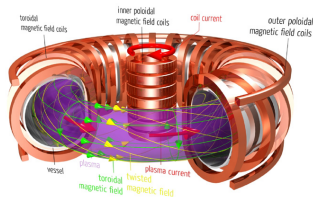
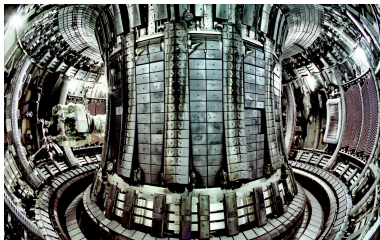
Figure: Adsorption process

Dispersion (column), diffusion (pellet) and non-linear adsorption (crystal)



Context, motivation

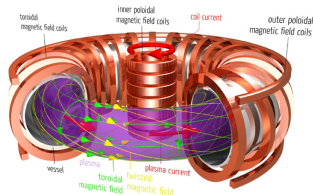
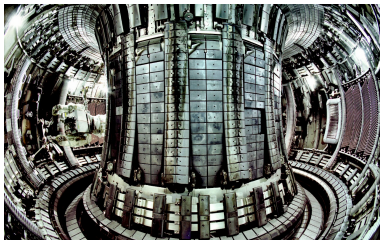
- Some examples of Distributed Parameter Systems for which the thermal domain plays a central role



- Several attempts have been made to extend port Hamiltonian and Lagrangian formulations to **Irreversible Thermodynamic systems**.

Context, motivation

- Some examples of Distributed Parameter Systems for which the thermal domain plays a central role



- Several attempts have been made to extend port Hamiltonian and Lagrangian formulations to **Irreversible Thermodynamic systems**.

In this talk ...

We present some results on the extension of PHS and IPHS formulations to infinite dimensional systems.

Context, motivation

We focus on systems defined on a one dimensional spatial domain.



Context, motivation

We focus on systems defined on a one dimensional spatial domain.

The aim is to generalize PHS formulations

$$\frac{\partial x}{\partial t} = \left(P_0 - G_0 + P_1 \frac{\partial}{\partial \zeta} \right) \mathcal{H}x(\zeta, t)$$

with

$$\begin{bmatrix} f_{\partial} \\ e_{\partial} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} P_1 & -P_1 \\ I & I \end{bmatrix} \begin{bmatrix} \mathcal{H}(b)x(b, t) \\ \mathcal{H}(a)x(a, t) \end{bmatrix} \quad (1)$$

to irreversible thermodynamic systems ...

????



1. Context, motivation
2. A simple but instructive example
3. Infinite dimensional irreversible port Hamiltonian systems (IPHS)
4. Conclusions



The isentropic fluid: the reversible case

We consider a **1-D isentropic fluid in Lagrangian coordinates**, also known as *p-system*, with $[a, b] \ni \zeta$, $a, b \in \mathbb{R}$, $a < b$. We choose as state variables

- ▶ the specific volume $\phi(\zeta, t)$,
- ▶ the velocity $v(\zeta, t)$ of the fluid.

System of two conservation laws :

$$\begin{aligned}\frac{\partial \phi}{\partial t}(\zeta, t) &= \frac{\partial v}{\partial \zeta}(\zeta, t) \\ \frac{\partial v}{\partial t}(\zeta, t) &= -\frac{\partial p}{\partial \zeta}(\zeta, t)\end{aligned}$$

where $p(\phi)$ is the pressure of the fluid. The total energy of the system is given by the sum of the kinetic energy and internal energy:

$$H(v, \phi) = \int_a^b \left(\frac{1}{2} v^2 + u(\phi) \right) dz$$

The isentropic fluid: the reversible case

The variational derivative of the total energy yields $\frac{\delta H}{\delta v} = v$ and $\frac{\delta H}{\delta \phi} = \frac{\partial u}{\partial \phi} = -p$ and the system may be written as the *Hamiltonian system*

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \end{bmatrix} = P_1 \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right), \quad \text{with} \quad P_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad (2)$$

Considering as input/output (W_B and W_C can be derived from P_1 [Le Gorrec et al., 2005]) :

$$\begin{bmatrix} v \\ y \end{bmatrix} = \begin{bmatrix} W_B \\ W_C \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta \phi}(b) \\ \frac{\delta H}{\delta \phi}(b) \\ \frac{\delta H}{\delta v}(a) \\ \frac{\delta H}{\delta v}(a) \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} -p(t, b) \\ v(t, b) \\ -p(t, a) \\ v(t, a) \end{bmatrix} = \begin{bmatrix} -p(t, b) \\ p(t, a) \\ v(t, b) \\ v(t, a) \end{bmatrix}$$

We have

$$\dot{H}(t) = y^\top(t)v(t)$$

The non-isentropic fluid: the irreversible case

We now consider some viscous damping τ . The momentum balance reads

$$\frac{\partial v}{\partial t}(\zeta, t) = -\frac{\partial p}{\partial \zeta}(\zeta, t) - \frac{\partial \tau}{\partial \zeta}(\zeta, t) \quad (3)$$

where

$$\tau = -\hat{\mu} \frac{\partial v}{\partial \zeta}$$

with $\hat{\mu}$ the viscous damping coefficient. It can be written as a dissipative port Hamiltonian system

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right) + \begin{bmatrix} 0 & 0 \\ 0 & \frac{\partial}{\partial \zeta} \left(\hat{\mu} \frac{\partial \cdot}{\partial \zeta} \right) \end{bmatrix} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right), \quad (4)$$

The non-isentropic fluid: the irreversible case

Splitting the dissipative operator we have

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right) + \begin{bmatrix} 0 \\ \frac{\partial}{\partial \zeta} \end{bmatrix} \hat{\mu} \begin{bmatrix} 0 & \frac{\partial}{\partial \zeta} \end{bmatrix} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right), \quad (5)$$

Which is equivalent to the DAE system:

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ f_e \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ e_e \end{bmatrix} \right), \quad (6)$$

with

$$e_e = \hat{\mu} f_e, \text{ with } \hat{\mu} > 0$$

The non-isentropic fluid: the irreversible case

Splitting the dissipative operator we have

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right) + \begin{bmatrix} 0 \\ \frac{\partial}{\partial \zeta} \end{bmatrix} \hat{\mu} \begin{bmatrix} 0 & \frac{\partial}{\partial \zeta} \end{bmatrix} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right), \quad (5)$$

Which is equivalent to the DAE system:

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \textcolor{blue}{f_e} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta \phi}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ \textcolor{red}{e_e} \end{bmatrix} \right), \quad (6)$$

with

$$\textcolor{red}{e_e} = \hat{\mu} \textcolor{blue}{f_e}, \text{ with } \hat{\mu} > 0$$

The existence of solutions can be proven based on the existence of solutions of the dissipation-free system by direct application of [Le Gorrec et al., 2005]



The non-isentropic fluid: the irreversible case

Splitting the dissipative operator we have

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right) + \begin{bmatrix} 0 \\ \frac{\partial}{\partial \zeta} \end{bmatrix} \hat{\mu} \begin{bmatrix} 0 & \frac{\partial}{\partial \zeta} \end{bmatrix} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \end{bmatrix} \right), \quad (5)$$

Which is equivalent to the DAE system:

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \underline{f_e} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \frac{\partial}{\partial \zeta} \left(\begin{bmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta \phi}{\delta H} \\ \underline{e_e} \end{bmatrix} \right), \quad (6)$$

with

$$\underline{e_e} = \hat{\mu} \underline{f_e}, \text{ with } \hat{\mu} > 0$$

The existence of solutions can be proven based on the existence of solutions of the dissipation-free system by direct application of [Le Gorrec et al., 2005] **but not stability**.

The non-isentropic fluid: the irreversible case

We can account for the **thermal domain** by considering Gibbs' equation

$$du = -pd\phi + Tds$$

where s denotes the entropy density and T the temperature. The total energy of the system is still the sum of the kinetic and the internal energy but now depends on **s**

$$H(v, \phi, \mathbf{s}) = \int_a^b \left(\frac{1}{2}v^2 + u(\phi, \mathbf{s}) \right) dz$$

From the conservation of the total energy and Gibbs' equation $\frac{\partial u}{\partial s} = T$ we get

$$\frac{\partial \mathbf{s}}{\partial t}(\zeta, t) = \frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right)^2(\zeta, t)$$

The non-isentropic fluid: the irreversible case

The system of balance equations may be written as the quasi-Hamiltonian system

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial(\cdot)}{\partial \zeta} & 0 \\ \frac{\partial(\cdot)}{\partial \zeta} & 0 & \frac{\partial}{\partial \zeta} \left(\frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) (\cdot) \right) \\ 0 & \frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) \frac{\partial(\cdot)}{\partial \zeta} & 0 \end{bmatrix} \begin{pmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ \frac{\delta H}{\delta s} \end{pmatrix}$$

Question: Is this operator formally skew symmetric ?

The non-isentropic fluid: the irreversible case

The system of balance equations may be written as the quasi-Hamiltonian system

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial(\cdot)}{\partial \zeta} & 0 \\ \frac{\partial(\cdot)}{\partial \zeta} & 0 & \frac{\partial}{\partial \zeta} \left(\frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) (\cdot) \right) \\ 0 & \frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) \frac{\partial(\cdot)}{\partial \zeta} & 0 \end{bmatrix} \begin{pmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ \frac{\delta H}{\delta s} \end{pmatrix}$$

Question: Is this operator formally skew symmetric ?

Question: Can you write down the energy balance ? What are the possible boundary port variables ?

The non-isentropic fluid: the irreversible case

The system of balance equations may be written as the quasi-Hamiltonian system

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial(\cdot)}{\partial \zeta} & 0 \\ \frac{\partial(\cdot)}{\partial \zeta} & 0 & \frac{\partial}{\partial \zeta} \left(\frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) (\cdot) \right) \\ 0 & \frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) \frac{\partial(\cdot)}{\partial \zeta} & 0 \end{bmatrix} \begin{pmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ \frac{\delta H}{\delta s} \end{pmatrix}$$

Question: Is this operator formally skew symmetric ?

Question: Can you write down the energy balance ? What are the possible boundary port variables ?

Question: Can you write down the entropy balance ? What are the possible boundary port variables ?

The non-isentropic fluid: the irreversible case

The system of balance equations may be written as the quasi-Hamiltonian system

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial(\cdot)}{\partial \zeta} & 0 \\ \frac{\partial(\cdot)}{\partial \zeta} & 0 & \frac{\partial}{\partial \zeta} \left(\frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) (\cdot) \right) \\ 0 & \frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) \frac{\partial(\cdot)}{\partial \zeta} & 0 \end{bmatrix} \begin{pmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ \frac{\delta H}{\delta s} \end{pmatrix}$$

Answer: Yes ! even if the differential operator is modulated.

The non-isentropic fluid: the irreversible case

The system of balance equations may be written as the quasi-Hamiltonian system

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial(\cdot)}{\partial \zeta} & 0 \\ \frac{\partial(\cdot)}{\partial \zeta} & 0 & \frac{\partial}{\partial \zeta} \left(\frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) (\cdot) \right) \\ 0 & \frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) \frac{\partial(\cdot)}{\partial \zeta} & 0 \end{bmatrix} \begin{pmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ \frac{\delta H}{\delta s} \end{pmatrix}$$

Answer: Yes ! even if the differential operator is modulated.

Answer: In case we do not have homogeneous BC:

$$\frac{dH}{dt} = y^T \nu$$

and

$$\frac{dS}{dt} = \int_a^b \sigma d\zeta \geq 0$$



1. Context, motivation
2. A simple but instructive example
3. Infinite dimensional irreversible port Hamiltonian systems (IPHS)
4. Conclusions



We introduce the Boundary Controlled Irreversible Port Hamiltonian System (BC-IPHS) defined on a 1D spatial domain $\zeta \in [a, b]$, $a, b \in \mathbb{R}$, $a < b$. The state variables of the system are the $n + 1$ *extensive variables*. The following partition of the state vector $\mathbf{x} \in \mathbb{R}^{n+1}$ shall be considered: the first n variables by $x = [q_1, \dots, q_n]^\top \in \mathbb{R}^n$ and the entropy density by $s \in \mathbb{R}$. Gibbs' equation is equivalent to the existence of an energy functional

$$H(x, s) = \int_a^b h(x(\zeta), s(\zeta)) d\zeta \quad (7)$$

where $h(x, s)$ is the energy density function. The total entropy functional is denoted by

$$S(t) = \int_a^b s(\zeta, t) d\zeta \quad (8)$$



IPHS : General formulation

An infinite dimensional IPHS undergoing m irreversible processes is defined by

$$\frac{\partial}{\partial t} \begin{bmatrix} x(\zeta, t) \\ s(\zeta, t) \end{bmatrix} = \begin{bmatrix} P_0 & G_0 \mathbf{R}_0 \\ -\mathbf{R}_0^\top G_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta x}(\zeta, t) \\ \frac{\delta H}{\delta s}(\zeta, t) \end{bmatrix} + \begin{bmatrix} P_1 \frac{\partial(\cdot)}{\partial \zeta} & \frac{\partial(G_1 \mathbf{R}_1 \cdot)}{\partial \zeta} \\ \mathbf{R}_1^\top G_1^\top \frac{\partial(\cdot)}{\partial \zeta} & g_s \mathbf{r}_s \frac{\partial(\cdot)}{\partial \zeta} + \frac{\partial(g_s \mathbf{r}_s \cdot)}{\partial \zeta} \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta x}(\zeta, t) \\ \frac{\delta H}{\delta s}(\zeta, t) \end{bmatrix} \quad (9)$$

where $P_0 = -P_0^\top \in \mathbb{R}^{n \times n}$, $P_1 = P_1^\top \in \mathbb{R}^{n \times n}$, $G_0 \in \mathbb{R}^{n \times m}$, $G_1 \in \mathbb{R}^{n \times m}$ with $m \leq n$ with $\mathbf{R}_l \left(\mathbf{x}, \frac{\delta H}{\delta \mathbf{x}} \right) \in \mathbb{R}^{m \times 1}$, $l = 0, 1$, defined by

$$R_{0,i} = \gamma_{0,i} \left(x, z, \frac{\delta H}{\delta x} \right) \{ S | G_0(:, i) | H \}$$

$$R_{1,i} = \gamma_{1,i} \left(x, z, \frac{\delta H}{\delta x} \right) \left\{ S | G_1(:, i) \frac{\partial}{\partial \zeta} | H \right\}$$

and

$$r_s = \gamma_s \left(x, z, \frac{\delta H}{\delta x} \right) \{ S | H \}$$

and $\gamma_{k,i} \left(x, z, \frac{\delta H}{\delta x} \right) > 0$, $k = 0, 1$; $i \in \{1, \dots, m\}$, $\gamma_s \left(x, z, \frac{\delta H}{\delta x} \right) > 0$ and $g_s(x)$,



For any two functionals H_1 and H_2 of the type (7) and for any matrix differential operator \mathcal{G} we define the pseudo-brackets

$$\begin{aligned}\{H_1|\mathcal{G}|H_2\} &= \begin{bmatrix} \frac{\delta H_1}{\delta \chi} \\ \frac{\delta H_1}{\delta s} \end{bmatrix} \begin{bmatrix} 0 & \mathcal{G} \\ -\mathcal{G}^* & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H_2}{\delta \chi} \\ \frac{\delta H_2}{\delta s} \end{bmatrix}, \\ \{H_1|H_2\} &= \frac{\delta H_1}{\delta s}^\top \left(\frac{\partial}{\partial \zeta} \frac{\delta H_2}{\delta s} \right)\end{aligned}\tag{10}$$

where \mathcal{G}^* denotes the formal adjoint operator of \mathcal{G} .



Remark 1:

Setting the matrices P_1 and G_1 to zero, reduces the PDE (11) to

$$\frac{d}{dt} \begin{bmatrix} x(\zeta, t) \\ s(\zeta, t) \end{bmatrix} = \begin{bmatrix} P_0 & G_0 \mathbf{R}_0(\mathbf{x}) \\ -\mathbf{R}_0(\mathbf{x})^\top G_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta \mathbf{x}}(\zeta, t) \\ \frac{\delta H}{\delta s}(\zeta, t) \end{bmatrix}$$

which is formally the definition of finite-dimensional IPHS in [Ramirez et al., 2013a, Ramirez et al., 2013b] for the case $m = 1$ or [Ramirez et al., 2014, Ramirez et al., 2016] for $m > 1$. In this sense the previous definition is an infinite-dimensional extension of the definition of IPHS.



Remark 1:

Setting the matrices P_1 and G_1 to zero, reduces the PDE (11) to

$$\frac{d}{dt} \begin{bmatrix} x(\zeta, t) \\ s(\zeta, t) \end{bmatrix} = \begin{bmatrix} P_0 & G_0 \mathbf{R}_0(\mathbf{x}) \\ -\mathbf{R}_0(\mathbf{x})^\top G_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta x}(\zeta, t) \\ \frac{\delta H}{\delta s}(\zeta, t) \end{bmatrix}$$

which is formally the definition of finite-dimensional IPHS in

[Ramirez et al., 2013a, Ramirez et al., 2013b] for the case $m = 1$ or

[Ramirez et al., 2014, Ramirez et al., 2016] for $m > 1$. In this sense the previous definition is an infinite-dimensional extension of the definition of IPHS.

Remark 2:

Setting the matrices G_0 and G_1 to zero reduces the PDE (11) to

$$\frac{d}{dt} \begin{bmatrix} x(\zeta, t) \\ s(\zeta, t) \end{bmatrix} = \begin{bmatrix} P_0 + P_1 \frac{\partial(\cdot)}{\partial \zeta} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta x}(\zeta, t) \\ \frac{\delta H}{\delta s}(\zeta, t) \end{bmatrix}$$

which is formally the definition of infinite-dimensional PHS.

Definition 1

A Boundary Controlled IPHS (BC-IPHS) is an infinite dimensional IPHS

$$\frac{\partial}{\partial t} \begin{bmatrix} x(\zeta, t) \\ s(\zeta, t) \end{bmatrix} = \begin{bmatrix} P_0 & G_0 \mathbf{R}_0 \\ -\mathbf{R}_0^\top G_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta \mathbf{x}}(\zeta, t) \\ \frac{\delta H}{\delta \mathbf{s}}(\zeta, t) \end{bmatrix} + \begin{bmatrix} P_1 \frac{\partial(\cdot)}{\partial \zeta} & \frac{\partial(G_1 \mathbf{R}_1 \cdot)}{\partial \zeta} \\ \mathbf{R}_1^\top G_1^\top \frac{\partial(\cdot)}{\partial \zeta} & g_s \mathbf{r}_s \frac{\partial(\cdot)}{\partial \zeta} + \frac{\partial(g_s \mathbf{r}_s \cdot)}{\partial \zeta} \end{bmatrix} \begin{bmatrix} \frac{\delta H}{\delta \mathbf{x}}(\zeta, t) \\ \frac{\delta H}{\delta \mathbf{s}}(\zeta, t) \end{bmatrix} \quad (11)$$

Augmented with the boundary port variables

$$v(t) = W_B \begin{bmatrix} e(t, b) \\ e(t, a) \end{bmatrix}, \quad y(t) = W_C \begin{bmatrix} e(t, b) \\ e(t, a) \end{bmatrix} \quad (12)$$

as linear functions of the modified effort variable

$$e(\zeta, t) = \begin{bmatrix} \frac{\delta H}{\delta \mathbf{x}}(\zeta, t) \\ \mathbf{R}(\mathbf{x}, \frac{\delta H}{\delta \mathbf{x}}) \frac{\delta H}{\delta \mathbf{s}}(\zeta, t) \end{bmatrix}, \text{ with } \mathbf{R} \left(\mathbf{x}, \frac{\delta H}{\delta \mathbf{x}} \right) = \begin{bmatrix} 1 & \mathbf{R}_1(\mathbf{x}, \frac{\delta \mathbf{H}}{\delta \mathbf{x}}) & \mathbf{r}_s(\mathbf{x}, \frac{\delta \mathbf{H}}{\delta \mathbf{x}}) \end{bmatrix}^\top \quad (13)$$

Furthermore

$$\begin{aligned} W_B &= \left[\frac{1}{\sqrt{2}} (\Xi_2 + \Xi_1 P_{ep}) M_p \quad \frac{1}{\sqrt{2}} (\Xi_2 - \Xi_1 P_{ep}) M_p \right], \\ W_C &= \left[\frac{1}{\sqrt{2}} (\Xi_1 + \Xi_2 P_{ep}) M_p \quad \frac{1}{\sqrt{2}} (\Xi_1 - \Xi_2 P_{ep}) M_p \right], \end{aligned}$$

where $M_p = (M^\top M)^{-1} M^\top$, $P_{ep} = M^\top P_e M$ and $M \in \mathbb{R}^{(n+m+2) \times k}$ is spanning the columns of $P_e \in \mathbb{R}^{n+m+2}$ of rank k , defined by

$$P_e = \begin{bmatrix} P_1 & 0 & G_1 & 0 \\ 0 & 0 & 0 & g_s \\ G_1^\top & 0 & 0 & 0 \\ 0 & g_s & 0 & 0 \end{bmatrix} \quad (14)$$

and where Ξ_1 and Ξ_2 in $\mathbb{R}^{k \times k}$ satisfy $\Xi_2^\top \Xi_1 + \Xi_1^\top \Xi_2 = 0$ and $\Xi_2^\top \Xi_2 + \Xi_1^\top \Xi_1 = I$.





First law of Thermodynamics

The total energy balance is

$$\dot{H} = y(t)^\top v(t)$$

which leads, when the input is set to zero, to $\dot{H} = 0$ in accordance with the first law of Thermodynamics.

Sketch of the proof

$$\frac{dH}{dt} = \int_a^b \begin{bmatrix} \frac{\delta H}{\delta x}^\top & \frac{\delta H}{\delta s} \end{bmatrix} \begin{bmatrix} \frac{dx}{dt} \\ \frac{ds}{dt} \end{bmatrix} d\zeta = \int_a^b \begin{bmatrix} \frac{\delta H}{\delta x}^\top & \frac{\delta H}{\delta s} \end{bmatrix} \mathcal{J}_e \begin{bmatrix} \frac{\delta H}{\delta x} \\ \frac{\delta H}{\delta s} \end{bmatrix} d\zeta = v^\top y$$



IPHS : General formulation

Second law of Thermodynamics

The total entropy balance is given by

$$\dot{S} = \int_a^b \sigma_t d\zeta + y_S^\top v_s$$

where y_s and v_s are the entropy conjugated input/output and σ_t is the total internal entropy production. This leads, when the input is set to zero, to $\dot{S} = \int_a^b \sigma_t d\zeta \geq 0$ in accordance with the second law of Thermodynamics.

Sketch of the proof

$$\begin{aligned}\dot{S} &= \int_a^b \frac{\partial S}{\partial t} d\zeta \\ &= \int_a^b \left(\mathbf{R}_0(\mathbf{x})^\top G_0^\top \frac{\delta H}{\delta x} + \mathbf{R}_1(\mathbf{x})^\top G_1^\top \frac{\partial}{\partial \zeta} \frac{\delta H}{\delta x} + \right. \\ &\quad \left. g_s \mathbf{r}_s(\mathbf{x}) \frac{\partial}{\partial \zeta} \frac{\delta H}{\delta s} + \frac{\partial}{\partial \zeta} \left(g_s \mathbf{r}_s(\mathbf{x}) \frac{\delta H}{\delta x} \right) \right) d\zeta \\ &= \int_a^b \sigma_t d\zeta - (f_s(b, t) - f_s(a, t))\end{aligned}$$

Back to 1D fluid



Recalling the 1D fluid model

$$\begin{bmatrix} \frac{\partial \phi}{\partial t} \\ \frac{\partial v}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & \frac{\partial(\cdot)}{\partial \zeta} & 0 \\ \frac{\partial(\cdot)}{\partial \zeta} & 0 & \frac{\partial}{\partial \zeta} \left(\frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) (\cdot) \right) \\ 0 & \frac{\hat{\mu}}{T} \left(\frac{\partial v}{\partial \zeta} \right) \frac{\partial(\cdot)}{\partial \zeta} & 0 \end{bmatrix} \begin{pmatrix} \frac{\delta H}{\delta \phi} \\ \frac{\delta H}{\delta v} \\ \frac{\delta H}{\delta s} \end{pmatrix}$$

$P_0 = 0, G_0 = 0, g_s = 0, P_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ and $G_1 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ with $x = \begin{bmatrix} \phi \\ v \end{bmatrix}$ and
 $R_{11} = \gamma_1 \{ S | G_1(:, 1) \frac{\partial}{\partial z} | H \}$ with $\gamma_1 = \frac{\hat{\mu}}{T} > 0$. In this case $n = 2, m = 1$



Back to 1D fluid

The boundary port variables may be computed as follows, starting with

$$P_e = \begin{bmatrix} P_1 & 0 & G_1 & 0 \\ 0 & 0 & 0 & g_s \\ G_1^\top & 0 & 0 & 0 \\ 0 & g_s & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

of rank $k = 2$ which gives $M = \begin{bmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}^\top$, $M_P = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \end{bmatrix}$ and

$P_{ep} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Choosing the parametrization

$$\Xi_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}, \quad \Xi_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix}$$

define the following boundary inputs and outputs

$$v(t) = \begin{bmatrix} -p(t, b) + \frac{\hat{\mu}}{T} \frac{\partial v}{\partial z}(t, b) \\ p(t, a) - \frac{\hat{\mu}}{T} \frac{\partial v}{\partial z}(t, a) \end{bmatrix}, \quad y(t) = \begin{bmatrix} v(t, b) \\ v(t, a) \end{bmatrix}.$$

1D fluid in Eulerian coordinates

If we now consider a **1-D isentropic fluid in Eulerian coordinates**, with $[a, b] \ni \zeta$, $a, b \in \mathbb{R}$, $a < b$. We choose as state variables

- ▶ the mass density $\rho(\zeta, t)$,
- ▶ the velocity $v(\zeta, t)$ of the fluid.

System of two conservation laws (coming from the use of material derivative $\frac{D}{Dt}(\cdot) = \frac{\partial}{\partial t}(\cdot) + v \frac{\partial}{\partial \zeta}(\cdot)$) and from Gibbs equation:

$$\frac{\partial \rho}{\partial t}(\zeta, t) = -\frac{\partial}{\partial \zeta}(\rho v)(\zeta, t)$$

$$\frac{\partial v}{\partial t}(\zeta, t) = -\frac{\partial}{\partial \zeta} \left(\frac{1}{2} v^2 + u + \frac{p}{\rho} \right)(\zeta, t) + \frac{T}{\rho} \frac{\partial s}{\partial \zeta}(\zeta, t) - \frac{1}{\rho} \frac{\partial}{\partial \zeta} \left(\frac{\tau}{\rho} \right)(\zeta, t)$$

and

$$\frac{\partial s}{\partial t}(\zeta, t) = -v \frac{\partial s}{\partial \zeta}(\zeta, t) - \frac{\tau}{\rho T} \frac{\partial v}{\partial \zeta}(\zeta, t)$$

1D fluid in Eulerian coordinates

Leading to the IPHS representation

$$\begin{bmatrix} \frac{\partial \rho}{\partial t} \\ \frac{\partial v}{\partial t} \\ \frac{\partial s}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 & -\frac{\partial(\cdot)}{\partial \zeta} & 0 \\ -\frac{\partial(\cdot)}{\partial \zeta} & 0 & 0 \\ 0 & -\frac{1}{\rho} \frac{\partial s}{\partial \zeta}(\zeta, t) + \frac{\mu}{\rho T} \frac{\partial v}{\partial \zeta} \frac{\partial}{\partial \zeta} \left(\frac{1}{\rho} \cdot \right) & 0 \end{bmatrix} \left(\frac{1}{\rho} \frac{\partial s}{\partial \zeta}(\zeta, t) + \frac{\mu}{\rho T} \frac{\partial v}{\partial \zeta} \left(\frac{\mu}{\rho T} \frac{\partial v}{\partial \zeta} \cdot \right) \right) \begin{bmatrix} \frac{\delta H}{\delta \rho} \\ \frac{\delta H}{\delta v} \\ \frac{\delta H}{\delta s} \end{bmatrix}$$

with

$$f_{\partial} = \begin{bmatrix} -v(b, t) \\ v(a, t) \end{bmatrix} \text{ and } e_{\partial} = \begin{bmatrix} \left(\rho \left(\frac{1}{2} v^2 + h \right) \right) (b, t) - \mu \frac{\partial v}{\partial \zeta} (b, t) \\ \left(\rho \left(\frac{1}{2} v^2 + h \right) \right) (a, t) - \mu \frac{\partial v}{\partial \zeta} (a, t) \end{bmatrix}$$

$$\text{and } h = u + \frac{p}{\rho}$$

Heat equation

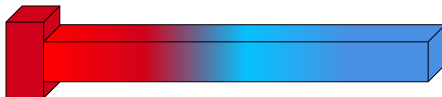


Figure: Heat conduction in a bar

Balance equation on u

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial \zeta} \left(-\lambda \frac{\partial T}{\partial \zeta} \right)$$

where λ denotes the heat conduction coefficient.

Question : Deduce from Gibbs' equation $du = Tds$ the IPHS formulation of the heat equation.



Heat equation

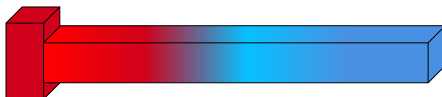


Figure: Heat conduction in a bar

Balance equation on u

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial \zeta} \left(-\lambda \frac{\partial T}{\partial \zeta} \right)$$

where λ denotes the heat conduction coefficient.

Question : Deduce from Gibbs' equation $du = Tds$ the IPHS formulation of the heat equation.

Question : Write the balance equation on the energy/entropy.



Heat equation

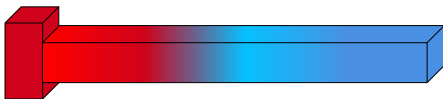


Figure: Heat conduction in a bar

Balance equation on u

$$\frac{\partial u}{\partial t} = -\frac{\partial}{\partial \zeta} \left(-\lambda \frac{\partial T}{\partial \zeta} \right)$$

where λ denotes the heat conduction coefficient. From Gibbs' equation $du = Tds$ and

$$\frac{\partial s}{\partial t} = -\frac{1}{T} \frac{\partial}{\partial \zeta} \left(-\lambda \frac{\partial T}{\partial \zeta} \right)$$

or alternatively

$$\frac{\partial s}{\partial t} = \frac{\partial}{\partial \zeta} \left(\frac{\lambda}{T} \frac{\partial T}{\partial \zeta} \right) + \frac{\lambda}{T^2} \left(\frac{\partial T}{\partial \zeta} \right)^2$$

One can notice that : $T = \frac{\delta U}{\delta s}$ where $U = \int_a^b u d\zeta$.

Heat equation

IPHS formulation

$$\frac{\partial s}{\partial t} = \frac{\lambda}{T^2} \frac{\partial T}{\partial \zeta} \frac{\partial}{\partial \zeta} \left(\frac{\delta U}{\delta s} \right) + \frac{\partial}{\partial \zeta} \left(\frac{\lambda}{T^2} \frac{\partial T}{\partial \zeta} \left(\frac{\delta U}{\delta s} \right) \right)$$

which is equivalent to (11) where $P_0 = 0$, $P_1 = 0$, $G_0 = 0$, $G_1 = 0$, $g_s = 1$ and $r_s = \gamma_s \{S|U\}$ with $\gamma_s = \frac{\lambda}{T^2}$ and $\{S|U\} = \frac{\partial T}{\partial \zeta}$. In this case $P_e = \frac{1}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $n = 1$ and $m = 1$. Choosing $\Xi_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix}$, $\Xi_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix}$ the boundary inputs and outputs of the system are

$$v(t) = \begin{bmatrix} \left(\frac{\lambda_s}{T} \frac{\partial T}{\partial \zeta} \right) (t, b) \\ - \left(\frac{\lambda_s}{T} \frac{\partial T}{\partial \zeta} \right) (t, a) \end{bmatrix}, \quad y(t) = \begin{bmatrix} T(t, b) \\ T(t, a) \end{bmatrix},$$

respectively the entropy flux and the temperature at each boundary.

Outline



Context, motivation

A simple but instructive example

Infinite dimensional irreversible port Hamiltonian systems (IPHS)

Conclusions





In this talk we have:

- ▶ introduced a new class of boundary controlled IPHS.
- ▶ illustrated it on some examples (fluid and heat equations).





In this talk we have:

- ▶ introduced a new class of boundary controlled IPHS.
- ▶ illustrated it on some examples (fluid and heat equations).

Current research lines:

- ▶ extend IPHS formulation to multidimensional systems such as fluids.
- ▶ extend the traditional control design techniques to thermally controlled BC-IPHS.
- ▶ use this formalism to overcome some traditional difficulties associated to irreversible Thermodynamics.





Thank you for your attention !





Le Gorrec, Y., Zwart, H., and Maschke, B. (2005).

Dirac structures and boundary control systems associated with skew-symmetric differential operators.
SIAM Journal on Control and Optimization, 44(5):1864–1892.



Ramirez, H., Le Gorrec, Y., Maschke, B., and Couenne, F. (2016).

On the passivity based control of irreversible processes: A port-Hamiltonian approach.
Automatica, 64:105 – 111.



Ramirez, H., Maschke, B., and Sbarbaro, D. (2013a).

Irreversible port-Hamiltonian systems: A general formulation of irreversible processes with application to the CSTR.
Chemical Engineering Science, 89(0):223 – 234.



Ramirez, H., Maschke, B., and Sbarbaro, D. (2013b).

Modelling and control of multi-energy systems: An irreversible port-Hamiltonian approach.
European Journal of Control, 19(6):513 – 520.



Ramirez, H., Sbarbaro, D., and Maschke, B. (2014).

Irreversible port-Hamiltonian formulation of chemical reaction networks.
In The 21st International Symposium on Mathematical Theory of Networks and Systems, Groningen, The Netherlands.

