Irreversible port-Hamiltonian systems: A framework for the modeling and control of thermodynamic systems.

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Spring School on Theory and Applications of Port-Hamiltonian Systems

Hector Ramirez and **Yann Le Gorrec**

Universidad Tecnica Federico Santa Maria, AC3E
Valparaiso, Chile.

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Supmicrotech, FEMTO-ST AS2M department
Besançon, France

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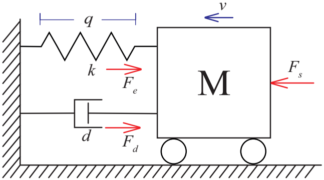
UNIVERSIDAD TECNICA
FEDERICO SANTA MARIA

AC3E
Advanced Center for Electrical
and Electronic Engineering

Outline

Brief intro on port-Hamiltonian systems

Some comments on modeling



The different forces acting on the mass are related by Newton's second law

$$F + F_d + F_e = F_s.$$

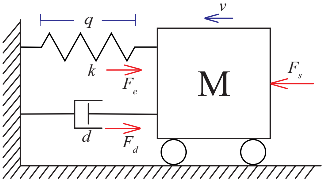
The constitutive laws of each element allows to write the forces in terms of internal variables, external inputs and the parameters. For linear relations $F = ma$, $F_e = kq$ and $F_d = dv$.

$$ma + dv + kq = F_s.$$

A dynamic model can be formulated defining a set of state variables. For instance the displacement q, then since $v = \dot{q}$ and $a = \ddot{q}$,

$$m\ddot{q} + d\dot{q} + kq = F_s,$$

which corresponds to a model of one ordinary differential equation (ODE) of order two.



Another alternative is to define as second state variable the velocity leading to a model of two ODEs of order one

$$\begin{aligned} \dot{q} &= v, \\ m\dot{v} + dv + kq &= F_s, \end{aligned}$$

which is well suited for *control* purposes. Indeed, define as state vector $x = [q, v]^\top$ and as controlled input the external force $u = F_s$, then the MSD system can be written as the linear control system

$$\dot{x} = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{d}{m} \end{bmatrix} x + \begin{bmatrix} 0 \\ \frac{1}{m} \end{bmatrix} u.$$

These are different models of the same system and each of them is valid under the performed assumption. The choice of one particular model will depend on the specific problem that needs to be studied.

Consider now the linear momentum $p = mv$ as state variable instead of the velocity then

$$\dot{p} = -kq - d\frac{p}{m} + F_s$$

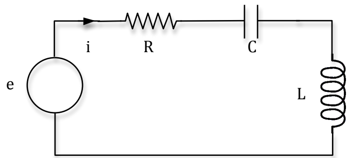
Defining as new state vector $x = [q, p]^\top$, the following dynamic model is obtained

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix}}_{J-D} \underbrace{\begin{bmatrix} kq \\ \frac{p}{m} \end{bmatrix}}_{\frac{\partial H}{\partial x}} + \underbrace{\begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{g} u$$

$$\underbrace{\dot{x}}_{f} = (J - D) \underbrace{\begin{bmatrix} F_e \\ v \end{bmatrix}}_{e} + g \underbrace{F_s}_{e_u}$$

There is a *structure* appearing related with the interconnection pattern of energy storing and energy dissipating elements, and that the change of the state variables (flows) in time is according to the structure and the *driving forces* (efforts). Furthermore, the dynamic model is directly related with the stored energy of the system

$$H(q, p) = \frac{1}{2}kq^2 + \frac{1}{2}\frac{p^2}{m}$$



Kirchhoff's law states sums of electrical currents at nodes are zero, and sums of voltages in closed loop must be zero.

$$V_r + V_L + V_C = V_e, \qquad i_r = i_L = i_C = i_e \tag{1}$$

The energy of the system is defined by the electric charge Q and the magnetic flux ϕ.

$$H(Q,\phi) = \frac{Q^2}{2C} + \frac{\phi^2}{2L}, \qquad \frac{\partial H}{\partial x} = \begin{bmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \phi} \end{bmatrix} = \begin{bmatrix} \frac{Q}{C} \\ \frac{\phi}{L} \end{bmatrix} = \begin{bmatrix} V_C \\ i_L \end{bmatrix},$$

The two energy-storing elements give rise to two linearly independent differential equations that characterize the dynamics of the energy variables.

$$\begin{aligned} i_C &= \dot{Q} = i_L = i_r = i_e, \\ V_L &= \dot{\phi} = -V_C - V_r + V_e. \end{aligned}$$

Using the constitutive relation of each element, the previous equations become

$$\dot{Q} = \frac{\phi}{L},$$
$$\dot{\phi} = -\frac{Q}{C} - r\frac{\phi}{L} + V_e,$$

where $V_r = ri_r$ with r is the resistance coefficient. Grouping terms with respect to the gradient of the energy and using the definition of the output of a port-Hamiltonian system, one has

$$\begin{bmatrix} \dot{Q} \\ \dot{\phi} \end{bmatrix} = \left(\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 0 & r \end{bmatrix} \right) \begin{bmatrix} \frac{Q}{C} \\ \frac{\phi}{L} \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} u,$$
$$y = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial Q} \\ \frac{\partial H}{\partial \phi} \end{bmatrix} = \frac{\phi}{L},$$

which is an input-output port-Hamiltonian system with

$$J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \text{and} \quad D = \begin{bmatrix} 0 & 0 \\ 0 & r \end{bmatrix}.$$

The matrix J, known as the *structure matrix*, embodies the energy-conserving interactions within the system. The matrix D represents the *dissipation matrix*, highlighting the presence of resistive elements. The PH framework facilitates the understanding of energy flow and the impact of different components on the system's behavior.

Port-Hamiltonian systems

An input-state-output port-Hamiltonian system with n-dimensional state space manifold $\mathcal{X}$, input and output spaces $U = Y = \mathbf{R}^m$, and Hamiltonian $H : \mathcal{X} \to \mathbf{R}$, is given as

$$\dot{x} = [J(x) - D(x)] \frac{\partial H}{\partial x}(x) + g(x)u$$
$$y = g^\top(x) \frac{\partial H}{\partial x}(x)$$

where the $n \times n$ matrices $J(x)$, $D(x)$ satisfy $J(x) = -J^\top(x)$ and $D(x) = D^\top(x) \geq 0$.

By the properties of $J(x)$, $D(x)$, it immediately follows that

$$\begin{aligned} \dot{H}(x(t)) &= \frac{\partial H}{\partial x}^\top \dot{x} \\ &= -\frac{\partial H}{\partial x}^\top D \frac{\partial H}{\partial x} + y^\top u \\ &\leq y^\top u \end{aligned}$$

implying passivity if $H \geq 0$. The Hamiltonian H is is equal to the total stored energy of the system, while $u^\top y$ is the externally supplied power.

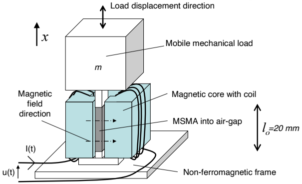
Context and motivation

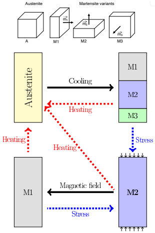
Motivations for adopting an energy-based perspective in modeling and control

- Physical system can be viewed as a set of simpler subsystems that exchange energy through ports,
- Energy is a concept common to all physical domains and is not restricted to linear or non-linear systems: non-linear approach,
- Energy can serve as a *lingua franca* to facilitate communication among scientists and engineers from different fields,
- Role of energy and the interconnections between subsystems provide the basis for various control techniques: Lyapunov based control.

Context and motivation

- Originating in macroscopic mechanics, port Hamiltonian formulations were proposed and intensively used for the modular modelling and control of conservative and dissipative multiphysics systems for which the thermal domain does not need to be explicitly represented.
- 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.





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

In this talk ...

We present some results on finite and infinite dimensional IPHS.

Context and motivation

(Dissipative-) Port Hamiltonian systems (PHS)

Class of non linear dynamic systems derived from an extension to open physical systems (1992) of Hamiltonian and Gradient systems. This class has been generalized (2001) to distributed parameter systems.

$$x(t):\begin{cases}\dot{x}=(J(x)-D(x))\,\frac{\partial H(x)}{\partial x}+B(x)u\\ y=B(x)^T\frac{\partial H(x)}{\partial x}\end{cases}\qquad x(t,z):\begin{cases}\dot{x}=(\mathcal{J}(x)-\mathcal{D}(x))\,\frac{\delta \mathcal{H}(x)}{\delta x}+\mathcal{B}_d u_d\\ y_d=\mathcal{B}_d^*\frac{\delta \mathcal{H}(x)}{\delta x}\\ \begin{pmatrix} f_\partial\\ e_\partial\end{pmatrix}=W\frac{\delta \mathcal{H}(x)}{\delta x}|_\partial,\end{cases}$$

$H(x)$ and $\mathcal{H}(x)$ are the Hamiltonian functions.

- In both cases the thermal domain is not accounted for and:

$$\frac{dH}{dt}\leq y^T u,\quad \text{or}\quad \frac{d\mathcal{H}}{dt}\leq y_d^T u_d+f_\partial^T e_\partial$$

- We show how this formalism can be generalized to cope with irreversible thermodynamic systems for which the thermal domain plays a central role : chemical reactors, reaction-diffusion systems, heat equation, temperature dependent systems such as smart materials, ...

Representation of irreversible Thermodynamic Systems

Several attempts have been made to extend port Hamiltonian and Lagrangian formulations to Irreversible Thermodynamic systems. Among others :

- metriplectic systems (sum of Hamiltonian and gradient systems) with one or two generating functions [Grmela and Öttinger, 1997, Grmela, 2002]
- control Hamiltonian systems defined on contact manifolds [Mrugala et al., 1991, Eberard et al., 2007, Favache et al., 2010, Ramirez et al., 2013] or their symplectization [van der Schaft and Maschke, 2018].
- pseudo-gradient systems [Favache et al., 2011],
- Irreversible/Thermodynamic port-Hamiltonian Systems and their control [Ramirez, 2012, Ramirez et al., 2016, Ramirez et al., 2022, Kirchhoff and Maschke, 2023, Maschke and Kirchhoff, 2023],
- constrained Lagrangian systems [Gay-Balmaz and Yoshimura, 2020, Gay-Balmaz and Yoshimura, 2023] which stem from variational principles.

Port-Hamiltonian systems (without dissipation)

[Maschke and van der Schaft, 1992, van der Schaft, 2000]

$$\dot{x} = J_0(x)\frac{\partial H_0}{\partial x}(x) + gu(t),$$
$$y = g(x)^\top \frac{\partial H_0}{\partial x}(x)$$

with H_0 the mechanical energy and $J_0(x) = -J_0(x)^\top$ the interconnection matrix

Balance equations expressed by PHS: Conservation of the **Hamiltonian**

$$\frac{dH_0}{dt} = \frac{\partial H_0}{\partial x}^\top gu = u^\top y$$

and of **Casimir's** of the Poisson bracket: $\{Z, G\}_{J_0} = \frac{\partial Z}{\partial x}^\top(x) J_0 \frac{\partial G}{\partial x}(x)$

$$\frac{dC}{dt} = \frac{\partial C}{\partial x}^\top gu = u^\top y_C$$

Thermodynamic systems

First and second laws of thermodynamics

Consider a closed system ($u = 0$),

$$\underbrace{\frac{dH_0}{dt} = 0}_{\text{First law}} \qquad \text{and} \qquad \underbrace{\frac{ds}{dt} = \sigma \geq 0}_{\text{Second law}}$$

$$\text{for PHS} \qquad \frac{ds}{dt} = \frac{\partial s}{\partial x}^\top J_0\left(x, \frac{\partial H_0}{\partial x}\right) \frac{\partial H_0}{\partial x} = \sigma \geq 0, \qquad \underline{\text{for any } H_0(x)}$$

This is the reason to consider quasi Hamiltonian system: retain much of the PHS structure, but their structure matrices depend explicitly on the gradient of the Hamiltonian (GENERIC, quasi Hamiltonian systems, Brayton-Mooser formulation,..)

[Grmela and Öttinger, 1997, Hangos et al., 2001, Otero-Muras et al., 2008, Eberard et al., 2007, Hoang et al., 2011, Favache and Dochain, 2010]

Thermodynamic system (dissipative PHS system)

$$\dot{x} = (J_0 - D_0)\frac{\partial H_0}{\partial x} + gu \qquad\qquad y = g^\top \frac{\partial H_0}{\partial x},$$

The energy balance is

$$\dot{H}_0 = -\frac{\partial H_0}{\partial x}^\top D_0 \frac{\partial H_0}{\partial x} + y^\top u,$$

If $D_0 \neq 0$ energy is being transformed into heat and the total energy is

$$H(x,s) = H_0(x) + U(s).$$

From the firs law if $u = 0$ the total energy has to be conserved

$$\dot{H} = -\frac{\partial H}{\partial x}^\top D_0 \frac{\partial H}{\partial x} + \frac{\partial U}{\partial s}\dot{s} = 0$$

From Gibbs' fundamental relation $T = \frac{\partial U}{\partial s} = \frac{\partial H}{\partial s}$, so the internal entropy creation is

$$\dot{s} = \frac{1}{T}\frac{\partial H}{\partial x}^\top D_0 \frac{\partial H}{\partial x} = \sigma \geq 0$$

in accordance with the second law of Thermodynamics.

The resulting system is then

$$\begin{bmatrix} \dot{x} \\ \dot{s} \end{bmatrix} = \begin{bmatrix} J_0 & -D_0 \frac{\partial H}{\partial x} \frac{1}{T} \\ \frac{1}{T} \frac{\partial H}{\partial x}^\top D_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial x} \\ T \end{bmatrix} + \begin{bmatrix} g \\ 0 \end{bmatrix} u,$$

$$y = \begin{bmatrix} g & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial x} \\ T \end{bmatrix}.$$

which corresponds to a quasi-Hamiltonian system [Ramirez et al., 2013]. In this sense the symplectic structure of the PHS, given by the Poisson tensor associated with the structure matrix is destroyed. **The structure matrix is co-state dependent!**

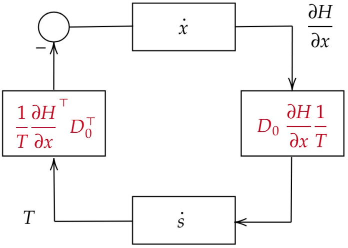
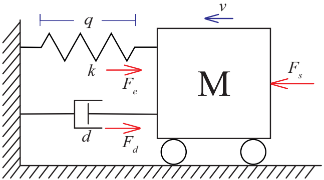


Figure: Quasi-Hamiltonian system

Implications

- Linearity between flows and efforts is lost. For a PHS the flows $\dot{x}$ and the efforts $\frac{\partial H_0}{\partial x}$ are related by a structure matrix (and eventually a dissipation matrix) which is constant or modulated by the state x.
- In control design the matching equations become in general harder to solve. Moreover in the case of control by interconnection, and in particular when making control design by energy shaping, the Casimir method needs to be rethought since the structure matrix depends on the energy.
- Structure preserving space discretization schemes for the case of infinite dimensional quasi-Hamiltonian systems need to be rethought [Cardoso-Ribeiro et al., 2024].

Entropy production of the MSD



PH model of the mass-spring-damper system

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix}}_{J-D} \underbrace{\begin{bmatrix} kq \\ \frac{p}{m} \end{bmatrix}}_{\frac{\partial H}{\partial x}} + \underbrace{\begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{g} u$$

$$\underbrace{\dot{x}}_{f} = (J-D) \underbrace{\begin{bmatrix} F_e \\ v \end{bmatrix}}_{e} + g \underbrace{F_s}_{e_u}$$

with energy function

$$H(q,p) = \frac{1}{2} kq^2 + \frac{1}{2} \frac{p^2}{m}$$

Entropy production of the MSD

Recall the dissipative PHS formulation of the MSD

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix}}_{J-R} \underbrace{\begin{bmatrix} kq \\ \frac{p}{m} \end{bmatrix}}_{\frac{\partial H}{\partial x}} + \underbrace{\begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{g} u, \qquad H_0(q,p) = \frac{1}{2}kq^2 + \frac{1}{2}\frac{p^2}{m}$$

If we would like to explicitly express the entropy balance due to the friction we can write the quasi-PHS

$$\begin{bmatrix} \dot{q} \\ \dot{p} \\ \dot{s} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & -d\frac{p}{m}\frac{1}{T} \\ 0 & d\frac{p}{m}\frac{1}{T} & 0 \end{bmatrix} \begin{bmatrix} kq \\ \frac{p}{m} \\ T \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} u,$$

$$y = \begin{bmatrix} g & 0 \end{bmatrix} \begin{bmatrix} kq \\ \frac{p}{m} \\ T \end{bmatrix}, \qquad \text{with} \quad H(x,s) = H(x) + U(s)$$

For many systems it is not necessary to take into account thermal domain. If temperature can be neglected then the PHS formulation is enough.

Some cases when temperature can not be neglected

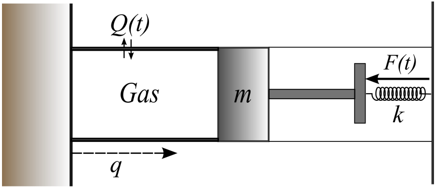


Figure: Gas piston system: a perfect gas contained in a cylinder enclosed by a moving piston.

The continuous stirred tank reactor (CSTR)

The chemical reaction is denoted by

$$\nu_1 A_1 + \ldots + \nu_{m-1} A_{m-1} \rightleftharpoons \nu_m A_m,$$

$\nu_1, \ldots, \nu_m$: stoichiometric coefficients
$A_1, \ldots, A_m$: chemical species

together with the definition of the reaction rate:

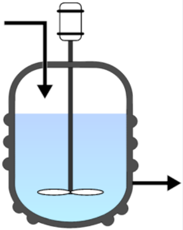
$$r(\mathcal{A}, T) = r_f(\mathcal{A}_f, T) - r_r(\mathcal{A}_f, T)$$

with $\mathcal{A}$ the affinity of reaction.

The mathematical model

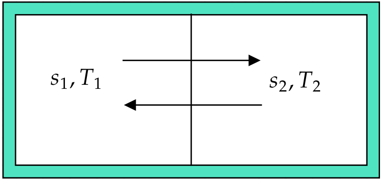
The balance equations [Aris, 1989],

$$\underbrace{\dot{n}_i = r_i V + F_{ei} - F_{si},}_{\text{mass}} \qquad \underbrace{\dot{S} = \sum_{i=1}^{m} (F_{ei} s_{ei} - F_{si} s_i) + \frac{Q}{T_w} + \sigma,}_{\text{entropy}}$$



The heat exchanger

The "simplest" thermodynamic system, i.e. the heat exchanger :



$$\dot{s}_1 = u_1 \qquad\qquad \dot{s}_2 = u_2$$

$$y_1 = \frac{\partial U_1}{\partial s_1} = T_1 \qquad\qquad y_2 = \frac{\partial U_2}{\partial s_2} = T_2$$

where s_1 and s_2 (resp. T_1 and T_2) are the entropies (resp. the temperatures) and U_1 and U_2 the internal energies of system 1 and 2. The inputs u_1 and u_2 correspond to the entropy flow that the systems exchange and y_1 and y_2 are the energy conjugated outputs.

Irreversible port-Hamiltonian systems

A non-linear extension of port Hamiltonian systems

Irreversible port Hamiltonian system (IPHS)

IPHS are a particular class of quasi-Hamiltonian systems. The state variables of the IPHS (for a simple thermodynamic system, i.e. uniform temperature) are the $n+1$ *extensive variables* of Thermodynamics (q_i plus s). From Gibb's equation

$$dH = Tds + \sum_{i=1}^{n} p_i dq_i$$

where T is the temperature, conjugated to the entropy, and the variables p_i denote the *intensive variables*, which are conjugated to the q_i extensive variables.

Definition (Poisson bracket)

For any two functions Z and G and for any matrix $\mathcal{G}$ we define the Poisson bracket as

$$\{Z, G\}_{J_\mathcal{G}} = \{Z|\mathcal{G}|G\} = \begin{bmatrix} \frac{\partial Z}{\partial x} \\ \frac{\partial Z}{\partial s} \end{bmatrix} \underbrace{\begin{bmatrix} 0 & \mathcal{G} \\ -\mathcal{G}^\top & 0 \end{bmatrix}}_{J_\mathcal{G}} \begin{bmatrix} \frac{\partial G}{\partial x} \\ \frac{\partial G}{\partial s} \end{bmatrix}$$

Simple IPHS

Definition

An IPHS undergoing j irreversible processes is defined by

- a pair of functions: the total energy $H : \mathbb{R}^{n+1} \to \mathbb{R}$ and the total entropy $s \in \mathbb{R}$,
- a pair of matrices $J_0 = -J_0^\top \in \mathbb{R}^{n\times n}$ and $G \in \mathbb{R}^{n\times j}$ with $j \leq n$ and the positive real-valued functions $\gamma_i\,(x, s)\,,\ i \in \{1, \ldots j\}$,

and the ODE

$$\begin{bmatrix} \dot{x} \\ \dot{s} \end{bmatrix} = \begin{bmatrix} J_0 & G\mathbf{R} \\ -\mathbf{R}^\top G^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial x} \\ \frac{\partial H}{\partial s} \end{bmatrix} + gu$$

$$y = g^\top \begin{bmatrix} \frac{\partial H}{\partial x} \\ \frac{\partial H}{\partial s} \end{bmatrix}$$

where $u, y \in \mathbb{R}^m$ are respectively the input and power conjugated output, and $g \in \mathbb{R}^{(n+1)\times m}$ the input map. The elements of the vector $\mathbf{R} \in \mathbb{R}^{j\times 1}$ are defined as

$$R_i = \gamma_i \left\{ s | G(:, i) | H \right\}$$

where the notation $G(:, i)$ indicates the i-th column of the matrix G.

IPHS

First law of Thermodynamics

The total energy balance is $\dot{H} = y^\top u$ implying that $\dot{H} = 0$ if $u = 0$ expressing the first law of Thermodynamics.

Second law of Thermodynamics

The internal entropy balance is given by the dynamic of the last coordinate with $u = 0$, which can be decomposed using the definition of $\mathbf{R}$ as

$$\dot{s} = -\mathbf{R}^\top G^\top \frac{\partial H}{\partial x} = -\sum_i^j \left(R_i G(:,i)^\top \frac{\partial H}{\partial x} \right)$$

$$= \sum_i^j \gamma_i \{s|G(:,i)|H\}^2 = \sum_i^j \sigma_i = \sigma \geq 0,$$

in accordance with the second law of Thermodynamics.

The continuous stirred tank reactor (CSTR)

The chemical reaction is denoted by

$$\nu_1 A_1 + \ldots + \nu_{m-1} A_{m-1} \rightleftharpoons \nu_m A_m,$$

$\nu_1, \ldots, \nu_m$: stoichiometric coefficients
$A_1, \ldots, A_m$: chemical species

together with the definition of the reaction rate:

$$r(\mathcal{A}, T) = r_f(\mathcal{A}_f, T) - r_r(\mathcal{A}_f, T)$$

with $\mathcal{A}$ the affinity of reaction.

The mathematical model

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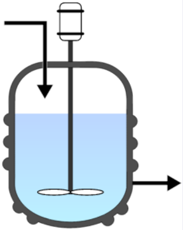


A single chemical reaction

$$\nu_1 A_1 + \ldots + \nu_{m-1} A_{m-1} \rightleftharpoons \nu_m A_m,$$

$\nu_1, \ldots, \nu_m$:	stoichiometric coefficients
$A_1, \ldots, A_m$:	chemical species
$\mathcal{A}$	affinity of reaction

together with the definition of the reaction rate:

$$r(\mathcal{A}, T) = r_f(\mathcal{A}, T) - r_r(\mathcal{A}, T)$$

$H = U$, the internal energy

$$\underbrace{G_r = \begin{bmatrix} \bar{\nu}_1 \\ \vdots \\ \bar{\nu}_m \end{bmatrix}}_{\text{stoichiometric vector}}, \qquad J_0 = 0, \qquad R = \frac{rV}{T}, \quad g = \begin{bmatrix} \mathbf{n_e} - \mathbf{n} & 0 \\ \phi\left(x, \frac{\partial U}{\partial x}\right) & \frac{1}{T_e} \end{bmatrix}, \qquad \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} \frac{F}{V} \\ Q \end{bmatrix}$$

$$\boxed{\{S, U\}_{J_R} = \mathcal{A} = -\sum_{i=1}^{m} \bar{\nu}_i \mu_i} \qquad \gamma = \frac{rV}{T\mathcal{A}} \geq 0,$$

$\mu_1, \ldots, \mu_m$:	chemical potentials
rV :	molar flow

Interconnection of simple IPHS

The general IPHS formulation

Interconnection of mechanical systems

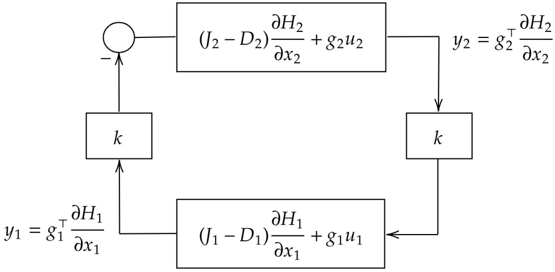


Figure: Feedback of PHS

Simple output feedback

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = k \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

where k is a constant.

Interconnection of mechanical systems

Consider the power-preserving interconnection law

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = k \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

where k is a constant. The closed-loop energy is then the sum of the stored energy in each system $H_0 = H_{0_1} + H_{0_2}$ and the total energy balance is

$$\begin{aligned} \dot{H}_0 &= -\frac{\partial H_{0_1}}{\partial x_1}^\top D_{0_1} \frac{\partial H_{0_1}}{\partial x_1} - \frac{\partial H_{0_2}}{\partial x_2}^\top D_{0_2} \frac{\partial H_{0_2}}{\partial x_2} + y_1^\top u_1 + y_2^\top u_2 \\ &= -\frac{\partial H_0}{\partial x}^\top \begin{bmatrix} D_{0_1} & 0 \\ 0 & D_{0_2} \end{bmatrix} \frac{\partial H_0}{\partial x} \leq 0 \end{aligned}$$

with $x = [x_1, x_2]^\top$. The closed-loop dynamics is given by

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = (J_0 - D_0) \begin{bmatrix} \frac{\partial H_{0_1}}{\partial x_1} \\ \frac{\partial H_{0_2}}{\partial x_2} \end{bmatrix} + \begin{bmatrix} g_1 & 0 \\ 0 & g_2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}, \qquad \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} g_1^\top & 0 \\ 0 & g_2^\top \end{bmatrix} \begin{bmatrix} \frac{\partial H_{0_1}}{\partial x_1} \\ \frac{\partial H_{0_2}}{\partial x_2} \end{bmatrix}$$

where the closed-loop interconnection and dissipation matrices are

$$J_0 = \begin{bmatrix} J_{0_1} & k g_1 g_2^\top \\ -k g_2 g_1^\top & J_{0_2} \end{bmatrix}, \qquad D_0 = \begin{bmatrix} D_{0_1} & 0 \\ 0 & D_{0_2} \end{bmatrix}$$

and where v_1 and v_2 are a new set of inputs. The resulting system is again a mechanical system.

The interconnection of thermodynamic systems

Assume for simplicity that a purely thermodynamic reservoir (s_1, T_1) is being interconnected with a purely mechanical system $\left(x_2, \frac{\partial H_2}{\partial x_2}\right)$ through some dissipative port and that the only source of entropy is the interconnection itself. Gibb's relation is then given by

$$\begin{aligned}\dot{H} &= T_1 \dot{s}_1 + \sum_{i=1}^{n} p_i \dot{q}_i \\ &= T_1 \dot{s}_1 + \frac{\partial H_2}{\partial x_2}^\top \dot{x}_2 \\ &= y_1^\top u_1 + y_2^\top u_2\end{aligned}$$

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = k \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

The previous power preserving interconnection assures energy conservation since $\dot{H} = 0$. Assuming uniform temperature, i.e. $T_1 = T$ and $s_1 = s$, the second law requires that $\dot{s} \geq 0$, or equivalently that

$$\dot{s} = -\frac{1}{T} \frac{\partial H_2}{\partial x_2}^\top \dot{x}_2 = -k \frac{1}{T} y_2^\top u_2 \geq 0$$

The interconnection law does **not** guarantee that this inequality holds

Proposition [Ramirez and Le Gorrec, 2024]

The power preserving interconnection of two thermodynamic systems needs to be **modulated** for the interconnected system to be a thermodynamic system. Furthermore, the modulating function depends on the the interface, input maps, the conjugated outputs (intensive variables) and the temperature of the systems.

Indeed, consider the modulated power preserving interconnection

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \beta \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

with β the modulating function. The entropy production becomes

$$\dot{s} = \beta \frac{1}{T} y_2^\top y_1 \geq 0 \quad \Rightarrow \quad \boxed{\beta = \gamma y_2^\top y_1, \ \gamma > 0 \quad \text{to satisfy the second law}}$$

The interconnection of thermodynamic systems

Similarly, if two thermodynamic reservoirs at different temperatures are interconnected, then the total entropy is

$$\dot{s} = \dot{s}_1 + \dot{s}_2 = \frac{\dot{H}_1}{T_1} + \frac{\dot{H}_2}{T_2} = \frac{T_2 \dot{H}_1 + T_1 \dot{H}_2}{T_1 T_2}$$

which requires that $\boxed{T_2 \dot{H}_1 + T_1 \dot{H}_2 \geq 0}$. Since $\dot{H}_i = y_i^\top u_i$, and using the modulated interconnection

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \beta \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

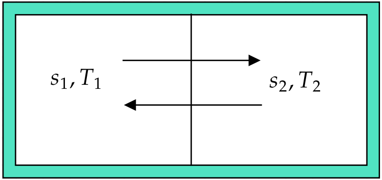
this condition becomes

$$\beta (T_2 - T_1) y_2^\top y_1 \geq 0 \quad \Rightarrow \quad \boxed{\beta = \gamma (T_2 - T_1) y_2^\top y_1}$$

The modulating function β is precisely defined by the ports of the systems, the temperature and the interface through the positive function γ.

The heat exchanger

The "simplest" thermodynamic system, i.e. the heat exchanger :



$$\dot{s}_1 = u_1 \qquad \dot{s}_2 = u_2$$

$$y_1 = \frac{\partial U_1}{\partial s_1} = T_1 \qquad y_2 = \frac{\partial U_2}{\partial s_2} = T_2$$

where s_1 and s_2 (resp. T_1 and T_2) are the entropies (resp. the temperatures) and U_1 and U_2 the internal energies of system 1 and 2. The inputs u_1 and u_2 correspond to the entropy flow that the systems exchange and y_1 and y_2 are the energy conjugated outputs.

The heat exchanger

According to Fourier's law the entropy flows into each subsystem are driven by the thermodynamic driving forces, which are the temperature differences between the compartments

$$u_1 = \frac{\lambda}{T_1}(T_2 - T_1) \qquad u_2 = \frac{\lambda}{T_2}(T_1 - T_2)$$

where $\lambda > 0$ denotes Fourier's heat conduction coefficient. According to the previous Proposition the previous relation can be equivalently written as

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \beta \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}$$

where $\beta = \frac{\lambda}{T_1 T_2}(T_2 - T_1)$. The interconnected system is then

$$\begin{bmatrix} \dot{s}_1 \\ \dot{s}_2 \end{bmatrix} = \frac{\lambda}{T_1 T_2}(T_2 - T_1) \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}$$
$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}$$

which is the IPHS model of the heat exchanger.

The heat exchanger

Consider in a second instance that the inputs are the heat flows rather than the entropy flows. The dynamical model of the heat exchanger is then

$$\dot{s}_i = \frac{1}{T_i} u_i, \qquad y_i = \frac{1}{T_i} \frac{\partial U_i}{\partial s_i} = 1$$

In this case the energy conjugated outputs are physically meaningless. The heat flow between the compartments are

$$u_1 = \lambda(T_2 - T_1) \qquad u_2 = \lambda(T_1 - T_2)$$

which can be equivalently written as

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \beta \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

with $\beta = \lambda(T_2 - T_1)$ in accordance with the previous Proposition. The interconnected system is then

$$\begin{bmatrix} \dot{s}_1 \\ \dot{s}_2 \end{bmatrix} = \frac{\lambda}{T_1 T_2}(T_2 - T_1) \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

which is the IPHS model of the heat exchanger.

Proposition [Ramirez and Le Gorrec, 2024]

Consider two IPHS, indexed by $i = 1, 2$, defined as

$$\begin{bmatrix} \dot{x}_i \\ \dot{s}_i \end{bmatrix} = J_i \begin{bmatrix} \frac{\partial H_i}{\partial x_i} \\ \frac{\partial H_i}{\partial s_i} \end{bmatrix} + g_i u_i, \qquad y_i = g_i^\top \begin{bmatrix} \frac{\partial H_i}{\partial x_i} \\ \frac{\partial H_i}{\partial s_i} \end{bmatrix}, \qquad \text{where} \qquad J_i = \begin{bmatrix} J_{0i} & G_i \mathbf{R}_i \\ -\mathbf{R}_i^\top G_i^\top & 0 \end{bmatrix}$$

with $x_i \in \mathbb{R}^{n_i}$, $s_i \in \mathbb{R}$, $u_i \in \mathbb{R}$, $J_{0_i} \in \mathbb{R}^{n_i \times n_i}$, $g_i \in \mathbb{R}^{(n_i+1)}$. Consider the modulated interconnection

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = R_u \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \qquad \text{where} \qquad R_u = \gamma_u \{ s | g_1 g_2^\top | H \}$$

with $s = s_1 + s_2$ and $H = H_1 + H_2$ the total entropy and the total energy.

The interconnection defines the IPHS

$$\begin{bmatrix} \dot{x}_1 \\ \dot{s}_1 \\ \dot{x}_2 \\ \dot{s}_2 \end{bmatrix} = J \begin{bmatrix} \frac{\partial H}{\partial x_1} \\ \frac{\partial H}{\partial s_1} \\ \frac{\partial H}{\partial x_2} \\ \frac{\partial H}{\partial s_2} \end{bmatrix} + g \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}, \qquad \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = g^\top \begin{bmatrix} \frac{\partial H}{\partial x_1} \\ \frac{\partial H}{\partial s_1} \\ \frac{\partial H}{\partial x_2} \\ \frac{\partial H}{\partial s_2} \end{bmatrix}, \qquad J = \begin{bmatrix} J_1 & R_u g_1 g_2^\top \\ -R_u g_2 g_1^\top & J_2 \end{bmatrix}$$

where $g = \begin{bmatrix} g_1 & 0 \\ 0 & g_2 \end{bmatrix}$, and v_1 and v_2 are a new set of inputs.

Comments

- The closed-loop system is obtained directly with the state modulated interconnection.
- Assume for simplicity $v_1 = v_2 = 0$. The structure matrix of the interconnected system J is skew-symmetric, hence $\dot{H} = 0 \Rightarrow$ conservation of the total Hamiltonian.

Corollary

The internal entropy production of the closed-loop system is $\sigma = \sigma_1 + \sigma_2 + \sigma_u \geq 0$, *where* σ_1 *and* σ_2 *are respectively the internal entropy production of system 1 and 2, and*

$$\sigma_u = \gamma_u \{s | g_1 g_2^\top | H\}^2 \geq 0$$

is the entropy produced by the interconnection of the systems.

(Proof sketch) Define $z = [x_1^\top, s_1, x_2^\top, s_2]^\top$, then $s = s_1 + s_2$,

$$\dot{s} = \frac{\partial s}{\partial z}^\top \dot{z} = \frac{\partial s}{\partial z}^\top J \frac{\partial H}{\partial z} = \frac{\partial s}{\partial z}^\top \left(J' + J_u \right) \frac{\partial H}{\partial z}$$
$$= \{s, H\}_{J'} + \{s, H\}_{J_u}$$

where

$$J' = \begin{bmatrix} J_1 & 0 \\ 0 & J_2 \end{bmatrix}, \quad \text{and} \quad J_u = \begin{bmatrix} 0 & R_u g_1 g_2^\top \\ -R_u g_2 g_1^\top & 0 \end{bmatrix}.$$

Developing the first bracket we obtain

$$\{s, H\}_{J'} = \begin{bmatrix} \frac{\partial s}{\partial x_1} \\ \frac{\partial s}{\partial s_1} \end{bmatrix}^\top J_1 \begin{bmatrix} \frac{\partial H}{\partial x_1} \\ \frac{\partial H}{\partial s_1} \end{bmatrix} + \begin{bmatrix} \frac{\partial s}{\partial x_2} \\ \frac{\partial s}{\partial s_2} \end{bmatrix}^\top J_2 \begin{bmatrix} \frac{\partial H}{\partial x_2} \\ \frac{\partial H}{\partial s_2} \end{bmatrix}$$
$$= -\mathbf{R_1}^\top G_1^\top \frac{\partial H_1}{\partial x_1} + -\mathbf{R_2}^\top G_2^\top \frac{\partial H_2}{\partial x_2} = \sigma_1 + \sigma_2 \geq 0$$

Developing the second bracket we obtain

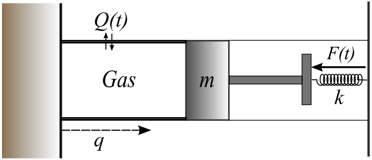
$$\{s, H\}_{J_u} = R_u \{s | g_1 g_2^\top | H\} = \gamma_u \{s | g_1 g_2^\top | H\}^2 = \sigma_u \geq 0$$

where σ_u is the entropy produced by the interconnection. The entropy balance is

$$\dot{s} = \sigma_1 + \sigma_2 + \sigma_u \geq 0$$

in accordance with the second law.

The gas-piston system (mechanical part)



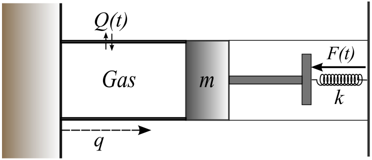
Consider an ideal gas contained in a cylinder enclosed by a moving piston which is attached to a spring. The system is characterized by the mechanical properties of the piston and the thermodynamic properties of the gas.

The mechanical energy of the piston is $H_0(q,p) = \frac{1}{2m}p^2 + \frac{1}{2}Kq^2$ and its PHS formulation

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} Kq \\ \frac{p}{m} \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} u_{p_1} \\ u_{p_2} \end{bmatrix}, \qquad \begin{bmatrix} y_{p_1} \\ y_{p_2} \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} Kq \\ \frac{p}{m} \end{bmatrix} = \begin{bmatrix} -v \\ v \end{bmatrix}$$

with $u_{p_1} = F_r$, $u_{p_2} = F_p$, q is the relative position of the spring, p is the momentum, $v = \frac{p}{m}$ is the velocity of the piston, $F = Kq$ is the force applied by the spring, F_p is the force applied on the piston by the gas pressure and F_r represents the mechanical friction with m the mass of the piston and K Hooke's constant.

The gas-piston system (thermodynamic part)



The internal energy of the perfect gas, $U(s,V)$, is a function of the entropy and the volume. The intensive variables of the gas are the temperature $T=\frac{\partial U}{\partial s}$ and the pressure $-P=\frac{\partial U}{\partial V}$. Furthermore, the temperature, the volume and the pressure of the gas are related by the law of the ideal gases $PV=rTN$, where N is the number of moles and r the ideal gas constant. The IPHS formulation of the gas is

$$\begin{bmatrix}\dot V\\ \dot s\end{bmatrix}=\begin{bmatrix}1&0\\0&1\end{bmatrix}\begin{bmatrix}u_1\\u_2\end{bmatrix},\qquad \begin{bmatrix}y_1\\y_2\end{bmatrix}=\begin{bmatrix}1&0\\0&1\end{bmatrix}\frac{\partial U}{\partial x}=\begin{bmatrix}-P\\T\end{bmatrix}$$

with $u_1=q_v$, $u_2=\sigma$, where V is the volume and s is the entropy of the gas, q_v is the gas flow due to the displacement of gas by the moving piston and σ is the irreversible creation of entropy due to the non-reversible transformation of mechanical friction into heat when the piston moves.

The gas-piston system (interconnection)

The piston and the gas are interconnected through a reversible and an irreversible relation.

Reversible interconnection

Relates the gas flow and the velocity of the piston and the pressure of the gas with the force applied on the piston. This interconnection can be formulated as the power preserving interconnection

$$\begin{bmatrix} u_1 \\ u_{p_2} \end{bmatrix} = A \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_{p_2} \end{bmatrix}$$

where A is the transversal area of the piston.

Irreversible interconnection

Relates the temperature of the gas with the mechanical friction force and the entropy creation with the velocity of the piston. The mechanical friction can be modeled as $F_r = bv$, and consequently the entropy creation is $\sigma = \frac{1}{T} bv^2$, with $b > 0$ the friction constant. The interconnection is formulated as

$$\begin{bmatrix} u_{p_1} \\ u_2 \end{bmatrix} = \underbrace{\frac{b}{T} v}_{\beta} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_{p_1} \\ y_2 \end{bmatrix}$$

The gas-piston system (IPHS formulation)

From the Proposition on interconnection of IPHS we have

$$\left\{ s \middle| \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} \middle| H \right\} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}^{\top} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} F \\ v \\ (-P) \\ T \end{bmatrix} = v$$

the velocity of the moving piston induces the heating of the gas and corresponds to the thermodynamic driving force of the interconnection. Consequently $\gamma = \frac{b}{T}$, $R = \beta = \frac{b}{T}v$.

IPHS formulation

Using the interconnections the gas-piston system is formulated as the IPHS

$$\begin{bmatrix} \dot{q} \\ \dot{p} \\ \dot{V} \\ \dot{s} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & A & -R \\ 0 & -A & 0 & 0 \\ 0 & R & 0 & 0 \end{bmatrix} \begin{bmatrix} F \\ v \\ (-P) \\ T \end{bmatrix}$$

The total energy of the system is the sum of the mechanical energy and the internal energy

$$H = H_0 + U = \frac{1}{2m}p^2 + \frac{1}{2}Kq^2 + U(s, V)$$

Some final remarks

- IPHS are thermodynamically coherent models which retain passivity features of PHS and satisfy the second law.
- The structure of IPHS has clear physical interpretation, characterizing the coupling between energy storing and energy dissipating elements, furthermore, the irreversible nature of the model is precisely expressed by the thermodynamic driving forces.
- Using the BC-IPHS formulation and motivated by PBC for BC-PHS on 1D spatial domains a BC that exponentially stabilizes the heat equation is proposed.
- The existence of structural invariant functions has been characterized in order to shape the closed-loop energy and assign the required closed-loop entropy.
- Future work aims to extend these control design techniques to a larger class of BC-IPHS such as reacting fluids and tubular reactors.

Thanks!

BC-IPHS

Boundary controlled IPHS with Yann Le Gorrec

An extension to distributed thermodynamical systems defined on one dimensional spatial domains

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