

Anisotropic heterogeneous n -D heat equation with boundary control and observation as port-Hamiltonian system: — Modeling & Discretization —

Denis MATIGNON

denis.matignon@isae.fr

Université de Toulouse, ISAE-SUPAERO, France

Joint work with: Anass SERHANI and Ghislain HAINE



INFIDHEM



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Introduction

- 1 Modeling:
 - Mathematical model: the Hamiltonian is a **quadratic** functional.
 - 1st thermodynamical model:
the Hamiltonian is the **entropy** S of the system.
 - 2nd thermodynamical model:
the Hamiltonian is the **internal energy** U of the system.
- 2 Discretization:
 - Use a Structure-Preserving Discretization taking advantage of the Finite Element Method: **PFEM** ("Partitioned Finite Element Method", see [Cardoso-Ribeiro, Matignon, Lefèvre, in proc. IFAC LHMNLC'2018]).
 - Perform simulation in an object-oriented environment, such as Python/FEniCS.

Overview

- 1 **Thermodynamical hypotheses**
- 2 **Lyapunov functional as Hamiltonian**
- 3 **Entropy as Hamiltonian**
- 4 **Energy as Hamiltonian**

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Thermodynamical hypotheses 1/2 Notations

- Spatial domain and physical parameters:
 - $\Omega \subset \mathbb{R}^{n \geq 1}$, a bounded open connected set.
 - $\vec{\mathbf{n}}$, the outward unit normal on the boundary $\partial\Omega$.
 - $\rho(\mathbf{x})$, the mass density.
 - $\overline{\overline{\lambda}}(\mathbf{x})$, the conductivity tensor.
- Notations:
 - T , the local temperature.
 - $\beta := \frac{1}{T}$, the reciprocal temperature.
 - u , the internal energy density.
 - s , the entropy density.
 - $\vec{\mathbf{J}}_Q$, the heat flux.
 - $\vec{\mathbf{J}}_S := \beta \vec{\mathbf{J}}_Q$, the entropy flux.
 - $C_V := \left(\frac{du}{dT} \right)_V$, the isochoric heat capacity.

Thermodynamical hypotheses 2/2 hypotheses

- **Assumption:** Constant volume and no chemical reaction.
- **1st law of thermodynamics:**

$$\rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) = -\operatorname{div} \left(\vec{\mathbf{J}}_Q(t, \mathbf{x}) \right).$$

- **Gibbs' relation:**

$$dU = T dS \quad \implies \quad \partial_t u(t, \mathbf{x}) = T(t, \mathbf{x}) \partial_t s(t, \mathbf{x}).$$

- **Entropy evolution:**

$$\rho(\mathbf{x}) \partial_t s(t, \mathbf{x}) = -\operatorname{div} \left(\vec{\mathbf{J}}_S(t, \mathbf{x}) \right) + \sigma(t, \mathbf{x}),$$

with $\sigma(t, \mathbf{x}) := \overrightarrow{\operatorname{grad}}(\beta) \cdot \vec{\mathbf{J}}_Q$, the irreversible entropy production.

- **Fourier's law:**

$$\vec{\mathbf{J}}_Q(t, \mathbf{x}) = -\overline{\lambda}(\mathbf{x}) \cdot \overrightarrow{\operatorname{grad}}(T(t, \mathbf{x})).$$

- **Dulong-Petit's law:** $u(t, \mathbf{x}) = C_V(\mathbf{x}) T(t, \mathbf{x})$.

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1 Thermodynamical hypotheses

2 **Lyapunov functional as Hamiltonian**

- Modeling
- Discretization
- Simulation

3 Entropy as Hamiltonian

4 Energy as Hamiltonian

Lyapunov functional - Modeling 1/3 quadratic Hamiltonian

Consider the **quadratic Hamiltonian**:

$$\mathcal{H}(t) := \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{C_V(t, \mathbf{x})} \, d\mathbf{x}$$

Choose u as energy variable, and compute the co-energy variable
 $\delta_u \mathcal{H} = \frac{u}{C_V}$, as variational derivative in L^2_{ρ} .

$$\begin{aligned} d_t \mathcal{H}(t) &= \int_{\Omega} \rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) \frac{u(t, \mathbf{x})}{C_V(t, \mathbf{x})} \, d\mathbf{x} - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{(C_V(t, \mathbf{x}))^2} \, d\mathbf{x}, \\ &= - \int_{\Omega} \operatorname{div} \left(\vec{\mathbf{J}}_{\mathcal{Q}}(t, \mathbf{x}) \right) \frac{u(t, \mathbf{x})}{C_V(t, \mathbf{x})} \, d\mathbf{x} - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{(C_V(t, \mathbf{x}))^2} \, d\mathbf{x}, \\ &= \int_{\Omega} \vec{\mathbf{J}}_{\mathcal{Q}}(t, \mathbf{x}) \cdot \overrightarrow{\operatorname{grad}} \left(\frac{u(t, \mathbf{x})}{C_V(t, \mathbf{x})} \right) \, d\mathbf{x} - \int_{\partial\Omega} \frac{u(t, \gamma)}{C_V(t, \gamma)} \vec{\mathbf{J}}_{\mathcal{Q}}(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma \\ &\quad - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) \frac{(u(t, \mathbf{x}))^2}{(C_V(t, \mathbf{x}))^2} \, d\mathbf{x}. \end{aligned}$$

Lyapunov functional - Modeling 2/3 port-Hamiltonian system

- Defining as flows and efforts:

$$f_u := \partial_t u, \quad e_u := \frac{u}{C_V}$$

$$\vec{f}_Q := -\overrightarrow{\mathbf{grad}} \left(\frac{u}{C_V} \right), \quad \vec{e}_Q := \vec{\mathbf{J}}_Q$$

- Port-Hamiltonian system:

$$\begin{pmatrix} \rho f_u \\ \vec{f}_Q \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\overrightarrow{\mathbf{grad}} & 0 \end{pmatrix} \begin{pmatrix} e_u \\ \vec{e}_Q \end{pmatrix}.$$

- Particular choices for **boundary control** v_∂ :
 - either the Dirichlet trace of e_u (temperature with Dulong-Petit),
 - or normal trace of $-\vec{e}_Q$ (inward heat flux).

Lyapunov functional - Modeling 3/3 power balance

- **Constitutive relations:**

- Dulong-Petit's law $\implies e_u = T$ and $\vec{f}_Q = -\overrightarrow{\text{grad}}(T)$
- Fourier's law $\implies \vec{e}_Q = -\bar{\lambda} \cdot \overrightarrow{\text{grad}}(T) \implies \vec{e}_Q = \bar{\lambda} \cdot \vec{f}_Q$

- **Power balance:**

$$d_t \mathcal{H}(t) = - \int_{\Omega} \vec{e}_Q(t, \mathbf{x}) \cdot \vec{f}_Q(t, \mathbf{x}) \, d\mathbf{x} + \int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) \, d\gamma - \frac{1}{2} \int_{\Omega} \rho(\mathbf{x}) \partial_t C_V(t, \mathbf{x}) (e_u(t, \mathbf{x}))^2 \, d\mathbf{x}$$

with the constitutive relations ($C_V(\mathbf{x})$ only):

$$d_t \mathcal{H}(t) = \underbrace{- \int_{\Omega} \vec{f}_Q(t, \mathbf{x}) \cdot \bar{\lambda} \cdot \vec{f}_Q(t, \mathbf{x}) \, d\mathbf{x}}_{\text{dissipation}} + \underbrace{\int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) \, d\gamma}_{\text{supplied power}}$$

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2 Lyapunov functional as Hamiltonian

- Modeling
- Discretization
- Simulation

3 Entropy as Hamiltonian

- Modeling
- Discretization
- Simulation

4 Energy as Hamiltonian

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Lyapunov functional - Discretization 1/4 weak form

- ① Weak form: Taking arbitrary test functions φ and $\vec{\varphi}$

$$\begin{cases} \int_{\Omega} \rho f_u \varphi \, d\mathbf{x} & = - \int_{\Omega} \operatorname{div}(\vec{e}_Q) \varphi \, d\mathbf{x}, \\ \int_{\Omega} \vec{f}_Q \cdot \vec{\varphi} \, d\mathbf{x} & = - \int_{\Omega} \overrightarrow{\operatorname{grad}}(e_u) \cdot \vec{\varphi} \, d\mathbf{x}. \end{cases}$$

For instance for the control of the inward heat flux $-\vec{e}_Q \cdot \vec{\mathbf{n}} = v_{\partial}$

- ② Apply Green's formula:

$$\begin{cases} \int_{\Omega} \rho f_u \varphi \, d\mathbf{x} & = \int_{\Omega} \vec{e}_Q \cdot \overrightarrow{\operatorname{grad}} \varphi \, d\mathbf{x} + \int_{\partial\Omega} v_{\partial} \varphi \, d\gamma, \\ \int_{\Omega} \vec{f}_Q \cdot \vec{\varphi} \, d\mathbf{x} & = - \int_{\Omega} \overrightarrow{\operatorname{grad}}(e_u) \cdot \vec{\varphi} \, d\mathbf{x}. \end{cases}$$

Lyapunov functional - Discretization 2/4 approximation bases

- *Finite-dimensional* bases:

$$\begin{aligned}\mathcal{X} &:= \text{span}\{\Phi\} := \text{span}\{(\varphi^i)_{1 \leq i \leq N}\}, \\ \mathcal{X} &:= \text{span}\{\vec{\Phi}\} := \text{span}\{(\vec{\varphi}^k)_{1 \leq k \leq \vec{N}}\}, \\ \mathcal{X}_\partial &:= \text{span}\{\Psi\} := \text{span}\{(\psi^m)_{1 \leq m \leq N_\partial}\},\end{aligned}$$

- Approximation:

$$\begin{aligned}f_u(t, \mathbf{x}) &\simeq f_u^d(t, \mathbf{x}) &:= \Phi^\top(\mathbf{x}) \cdot \underline{f}_u(t) &:= \sum_{i=1}^N f_u^i(t) \varphi^i(\mathbf{x}) \\ \vec{f}_Q(t, \mathbf{x}) &\simeq \vec{f}_Q^d(t, \mathbf{x}) &:= \vec{\Phi}^\top(\mathbf{x}) \cdot \vec{\underline{f}}_Q(t) &:= \sum_{k=1}^{\vec{N}} \vec{f}_Q^k(t) \vec{\varphi}^k(\mathbf{x}) \\ v_\partial(t, \gamma) &\simeq v_\partial^d(t, \gamma) &:= \psi_\partial^\top(\gamma) \cdot \underline{v}_\partial(t) &:= \sum_{m=1}^{N_\partial} v_\partial^m(t) \psi_\partial^m(\mathbf{x})\end{aligned}$$

and similarly for the other variables.

Lyapunov functional - Discretization 3/4 matrix form

The discrete weak formulation on $\mathcal{X} \times \mathcal{X} \times \mathcal{X}_\partial$ reads:

$$\begin{cases} M_\rho \underline{f}_u(t) &= D \underline{e}_Q(t) + B \underline{v}_\partial(t), \\ \vec{M} \underline{f}_Q(t) &= -D^\top \underline{e}_u(t), \\ M_\partial \underline{y}_\partial(t) &= B^\top \underline{e}_u(t), \end{cases}$$

with the following sparse matrices:

$$\begin{aligned} M_\rho &:= \int_\Omega \Phi \cdot \Phi^\top \rho \, d\mathbf{x} \in \mathbb{R}^{N \times N}, \quad \vec{M} := \int_\Omega \vec{\Phi} \cdot \vec{\Phi}^\top \, d\mathbf{x} \in \mathbb{R}^{\vec{N} \times \vec{N}}, \\ D &:= \int_\Omega \mathbf{grad}(\Phi) \cdot \vec{\Phi}^\top \, d\mathbf{x} \in \mathbb{R}^{N \times \vec{N}}, \quad B := \int_{\partial\Omega} \Phi \cdot \Psi^\top \, d\gamma \in \mathbb{R}^{N \times N_\partial} \\ M_\partial &:= \int_{\partial\Omega} \Psi \cdot \Psi^\top \, d\gamma \in \mathbb{R}^{N_\partial \times N_\partial}. \end{aligned}$$

Compact form:

$$\underbrace{\begin{pmatrix} M_\rho & 0 & 0 \\ 0 & \vec{M} & 0 \\ 0 & 0 & M_\partial \end{pmatrix}}_{\mathcal{M}_d} \underbrace{\begin{pmatrix} \underline{f}_u(t) \\ \underline{f}_Q(t) \\ -\underline{y}_\partial(t) \end{pmatrix}}_{\vec{f}_d} = \underbrace{\begin{pmatrix} 0 & D & B \\ -D^\top & 0 & 0 \\ -B^\top & 0 & 0 \end{pmatrix}}_{\mathcal{J}_d} \underbrace{\begin{pmatrix} \underline{e}_u(t) \\ \underline{e}_Q(t) \\ \underline{v}_\partial(t) \end{pmatrix}}_{\vec{e}_d}$$

Lyapunov functional - Discretization 4/4 structure

- **Structure-preservation:** $\vec{e}_d^\top \mathcal{M}_d \vec{f}_d = 0$ (thanks to $\mathcal{J}_d = -\mathcal{J}_d^*$)
- **Discrete closure relations:**

- Dulong-Petit's law:

$$\int_{\Omega} \rho C_V \partial_t e_u \varphi \, dx = \int_{\Omega} \rho f_u \varphi \, dx \implies M_{\rho C_V} \frac{d}{dt} \underline{e}_u = M_{\rho} \underline{f}_u,$$

- Fourier's law:

$$\int_{\Omega} \vec{e}_Q \cdot \vec{\varphi} \, dx = \int_{\Omega} (\bar{\lambda} \cdot \vec{f}_Q) \cdot \vec{\varphi} \, dx \implies \vec{M} \underline{e}_Q = \vec{\Lambda} \underline{f}_Q$$

- **Discrete Hamiltonian:**

$$\mathcal{H}_d(t) = \frac{1}{2} \underline{e}_u^\top(t) M_{\rho C_V} \underline{e}_u(t)$$

- **Discrete power balance:**

$$d_t \mathcal{H}_d(t) = \underbrace{-\vec{f}_Q^\top(t) \vec{\Lambda} \vec{f}_Q(t)}_{\text{discrete dissipation}} + \underbrace{\underline{v}_Q^\top(t) M_{\partial} \underline{y}_Q(t)}_{\text{discrete supplied power}}$$

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- Modeling
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3 Entropy as Hamiltonian

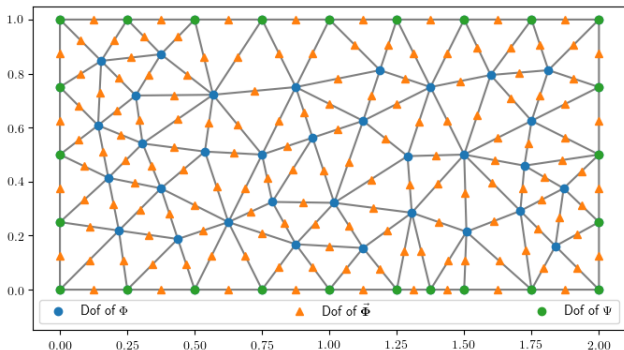
- Modeling
- Discretization
- Simulation

4 Energy as Hamiltonian

- Modeling
- Discretization
- Simulation

Lyapunov functional - Simulation ^{1/2}

- Domain: $\Omega = (0, L_x) \times (0, L_y)$ with $L_x = 2$ and $L_y = 1$.
- Finite element: $\mathcal{X} \times \mathcal{X} \times \mathcal{X}_\partial = \mathbf{P}_1 \times \mathbf{RT}_0 \times \gamma_0(\mathbf{P}_1)$



$$\rho(\mathbf{x}) := x_1(2 - x_1) + 1, \quad C_V = 3, \quad \bar{\lambda}(\mathbf{x}) = \begin{pmatrix} 5 + x_1x_2 & (x_1 - x_2)^2 \\ (x_1 - x_2)^2 & 3 + \frac{x_2}{x_1 + 1} \end{pmatrix}$$

Lyapunov functional - Simulation 2/2 time-space simulation

What about... thermodynamics?

- 1 Read *Distributed port-Hamiltonian modelling for irreversible processes*, by W. Zhou, B. Hamroun, F. Couenne, Y. Le Gorrec. in *Mathematical and Computer Modelling of Dynamical Systems*, vol. 23, n. 1, 2017.
- 2 Have the chance to talk with Françoise Couenne (LAGEP).

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1 Thermodynamical hypotheses

2 Lyapunov functional as Hamiltonian

3 Entropy as Hamiltonian

- Modeling
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- Simulation

4 Energy as Hamiltonian

Entropy functional - Modeling 1/3 Hamiltonian Entropy

Consider the **entropy** of the system as **Hamiltonian**:

$$S(t) := \int_{\Omega} \rho(\mathbf{x}) s(u(t, \mathbf{x})) \, d\mathbf{x},$$

Choose u as energy variable, and compute the co-energy variable

$$\delta_u S = \frac{ds}{du} = \beta.$$

$$\begin{aligned} d_t S(t) &= \int_{\Omega} \rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) \beta(t, \mathbf{x}) \, d\mathbf{x}, \\ &= \int_{\Omega} \rho(\mathbf{x}) \partial_t s(t, \mathbf{x}) \, d\mathbf{x}, \\ &= - \int_{\Omega} \operatorname{div} \left(\vec{\mathbf{J}}_S(t, \mathbf{x}) \right) \, d\mathbf{x} + \int_{\Omega} \sigma(t, \mathbf{x}) \, d\mathbf{x}, \\ &= - \int_{\partial\Omega} \vec{\mathbf{J}}_S(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma + \int_{\Omega} \sigma(t, \mathbf{x}) \, d\mathbf{x}, \\ &= - \int_{\partial\Omega} \beta(t, \gamma) \vec{\mathbf{J}}_Q(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma + \int_{\Omega} \sigma(t, \mathbf{x}) \, d\mathbf{x}. \end{aligned}$$

Entropy functional - Modeling 2/3 port-Hamiltonian system

- Defining as *flows* and *efforts*:

$$\begin{aligned} f_u &:= \partial_t u, & e_u &:= \beta \\ \vec{f}_Q &:= -\mathbf{grad}(\beta), & \vec{e}_Q &:= \vec{J}_Q \end{aligned}$$

- Port-Hamiltonian system:

$$\begin{pmatrix} \rho f_u \\ \vec{f}_Q \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\mathbf{grad} & 0 \end{pmatrix} \begin{pmatrix} e_u \\ \vec{e}_Q \end{pmatrix}.$$

- Particular choices for boundary control v_∂ :
 - either the Dirichlet trace of e_u (reciprocal temperature),
 - or normal trace of $-\vec{e}_Q$ (inward heat flux).

Entropy functional - Modeling 3/3 power balance

- Constitutive relations:

- Dulong-Petit's law: $u = \frac{C_V}{\beta} \implies e_u = \frac{C_V}{u}$

- Fourier's law: $\vec{e}_Q = \frac{1}{\beta^2} \bar{\lambda} \cdot \overrightarrow{\text{grad}}(\beta) \implies \vec{e}_Q = -\frac{1}{e_u^2} \bar{\lambda} \cdot \vec{f}_Q$

- Power balance:

$$d_t S(t) = - \int_{\Omega} \vec{f}_Q(t, \mathbf{x}) \cdot \vec{e}_Q(t, \mathbf{x}) \, d\mathbf{x} + \int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) \, d\gamma.$$

with the constitutive relations:

$$d_t S(t) = \underbrace{\int_{\Omega} \sigma(t, \mathbf{x}) \, d\mathbf{x}}_{\substack{\text{entropy production} \\ \geq 0}} + \underbrace{\int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) \, d\gamma}_{\text{supplied part}}$$

Entropy functional - Discretization 1/3 weak form

- ① Weak form: Taking arbitrary test functions φ and $\vec{\varphi}$

$$\begin{cases} \int_{\Omega} \rho f_u \varphi \, d\mathbf{x} & = - \int_{\Omega} \operatorname{div}(\vec{e}_Q) \varphi \, d\mathbf{x}, \\ \int_{\Omega} \vec{f}_Q \cdot \vec{\varphi} \, d\mathbf{x} & = - \int_{\Omega} \overrightarrow{\operatorname{grad}}(e_u) \cdot \vec{\varphi} \, d\mathbf{x}. \end{cases}$$

For instance for the control of the inward heat flux $-\vec{e}_Q \cdot \vec{\mathbf{n}} = v_{\partial}$

- ② Apply Green's formula:

$$\begin{cases} \int_{\Omega} \rho f_u \varphi \, d\mathbf{x} & = \int_{\Omega} \vec{e}_Q \cdot \overrightarrow{\operatorname{grad}} \varphi \, d\mathbf{x} + \int_{\partial\Omega} v_{\partial} \varphi \, d\gamma, \\ \int_{\Omega} \vec{f}_Q \cdot \vec{\varphi} \, d\mathbf{x} & = - \int_{\Omega} \overrightarrow{\operatorname{grad}}(e_u) \cdot \vec{\varphi} \, d\mathbf{x}. \end{cases}$$

Entropy functional - Discretization 2/3 matrix form

The discrete system:

$$\begin{cases} M_\rho \underline{f}_u(t) &= D \underline{e}_Q(t) + B \underline{v}_\partial(t), \\ \vec{M} \underline{f}_Q(t) &= -D^\top \underline{e}_u(t), \\ M_\partial \underline{y}_\partial(t) &= B^\top \underline{e}_u(t), \end{cases}$$

$$\begin{aligned} M_\rho &:= \int_\Omega \Phi \cdot \Phi^\top \rho \, d\mathbf{x} \in \mathbb{R}^{N \times N}, \quad \vec{M} := \int_\Omega \vec{\Phi} \cdot \vec{\Phi}^\top \, d\mathbf{x} \in \mathbb{R}^{\vec{N} \times \vec{N}}, \\ D &:= \int_\Omega \mathbf{grad}(\Phi) \cdot \vec{\Phi}^\top \, d\mathbf{x} \in \mathbb{R}^{N \times \vec{N}}, \quad B := \int_{\partial\Omega} \Phi \cdot \Psi^\top \, d\gamma \in \mathbb{R}^{N \times N_\partial} \\ M_\partial &:= \int_{\partial\Omega} \Psi \cdot \Psi^\top \, d\gamma \in \mathbb{R}^{N_\partial \times N_\partial}. \end{aligned}$$

Compact form:

$$\underbrace{\begin{pmatrix} M_\rho & 0 & 0 \\ 0 & \vec{M} & 0 \\ 0 & 0 & M_\partial \end{pmatrix}}_{\mathcal{M}_d} \underbrace{\begin{pmatrix} \underline{f}_u(t) \\ \underline{f}_Q(t) \\ -\underline{y}_\partial(t) \end{pmatrix}}_{\vec{f}_d} = \underbrace{\begin{pmatrix} 0 & D & B \\ -D^\top & 0 & 0 \\ -B^\top & 0 & 0 \end{pmatrix}}_{\mathcal{J}_d} \underbrace{\begin{pmatrix} \underline{e}_u(t) \\ \underline{e}_Q(t) \\ \underline{v}_\partial(t) \end{pmatrix}}_{\vec{e}_d}$$

Entropy functional - Discretization 3/3 structure

- **Structure-preservation:** $\vec{e}_d^\top \mathcal{M}_d \vec{f}_d = 0$ (thanks to $\mathcal{J}_d = -\mathcal{J}_d^*$)
- **Discrete closure relations:**

- Dulong-Petit's law:

$$\int_{\Omega} \rho \beta \varphi \, d\mathbf{x} = \int_{\Omega} \rho \frac{C_V}{u} \varphi \, d\mathbf{x} \implies \text{(1st Non-linear closure equation),}$$

- Fourier's law:

$$\int_{\Omega} \vec{e}_Q \cdot \vec{\varphi} \, d\mathbf{x} = - \int_{\Omega} \frac{1}{e_u^2} \vec{f}_Q \cdot \vec{\lambda} \cdot \vec{\varphi} \, d\mathbf{x} \implies \text{(2nd Non-linear closure eqn.)}$$

- **Discrete power balance:**

$$d_t S_d(t) = \underbrace{-\vec{f}_Q^\top(t) \vec{M} \vec{e}_Q(t)}_{\text{discrete entropy production}} + \underbrace{\underline{v}_\partial^\top(t) M_\partial \underline{y}_\partial(t)}_{\text{discrete supplied power}} \geq 0$$

Entropy functional - Simulation ^{1/}

Overview

- 1 Thermodynamical hypotheses
- 2 Lyapunov functional as Hamiltonian
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- 4 Energy as Hamiltonian**
 - Modeling
 - Discretization
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Energy functional - Modeling

Consider the **internal energy** of the system as **Hamiltonian**:

$$U(t) := \int_{\Omega} \rho(\mathbf{x}) u(s(t, \mathbf{x})) \, d\mathbf{x},$$

Choosing s as energy variable, compute the co-energy variable

$$\delta_s U = \frac{du}{ds} = T.$$

$$\begin{aligned} d_t U(t) &= \int_{\Omega} \rho(\mathbf{x}) \partial_t s(t, \mathbf{x}) T(t, \mathbf{x}) \, d\mathbf{x}, \\ &= \int_{\Omega} \rho(\mathbf{x}) \partial_t u(t, \mathbf{x}) \, d\mathbf{x}, \\ &= - \int_{\Omega} \operatorname{div} \left(\vec{\mathbf{J}}_Q(t, \mathbf{x}) \right) \, d\mathbf{x}, \\ &= - \int_{\partial\Omega} \vec{\mathbf{J}}_Q(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma, \\ &= - \int_{\partial\Omega} T(t, \gamma) \vec{\mathbf{J}}_S(t, \gamma) \cdot \vec{\mathbf{n}}(\gamma) \, d\gamma. \end{aligned}$$

Energy functional - Modeling 2/3 port-Hamiltonian system

- Defining as *flows* and *efforts*:

$$\begin{aligned} f_s &:= \partial_t s, & e_u &:= T \\ \vec{f}_s &:= -\overrightarrow{\mathbf{grad}}(T), & \vec{e}_s &:= \vec{\mathbf{J}}_s \end{aligned}$$

- Primary port-Hamiltonian system:

$$\begin{pmatrix} \rho f_u \\ \vec{f}_Q \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} \\ -\overrightarrow{\mathbf{grad}} & 0 \end{pmatrix} \begin{pmatrix} e_u \\ \vec{e}_Q \end{pmatrix} + \begin{pmatrix} \sigma \\ 0 \end{pmatrix}.$$

- Following [Zhou & al., 2017], we introduced new ports:

$$f_\sigma = T, \quad e_\sigma = -\sigma$$

- Port-Hamiltonian system

$$\begin{pmatrix} \rho f_u \\ \vec{f}_Q \\ f_\sigma \end{pmatrix} = \begin{pmatrix} 0 & -\text{div} & -1 \\ -\overrightarrow{\mathbf{grad}} & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} e_u \\ \vec{e}_Q \\ e_\sigma \end{pmatrix}.$$

Entropy functional - Modeling 3/3 power balance

- Particular choices for boundary control v_{∂} :
 - either the Dirichlet trace of e_s (temperature),
 - or normal trace of $-\vec{e}_s$ (inward entropy flux).
- Constitutive relations:
 - Dulong-Petit's law and Gibbs' relation:
 $C_V \rho \partial_t T = T \rho \partial_t s \implies C_V \rho \partial_t e_s = e_s f_s$
 - Fourier's law: $e_s \vec{e}_s = \bar{\lambda} \cdot \vec{f}_s$
 - Entropy closure relation: $\vec{f}_s \cdot \vec{e}_s + f_\sigma e_\sigma = 0$
- Power balance:

$$d_t U(t) = \int_{\partial\Omega} v_{\partial}(t, \gamma) y_{\partial}(t, \gamma) \, d\gamma$$

Entropy functional - Discretization 1/3 weak form

- ① Weak form: Taking arbitrary test functions φ and $\vec{\varphi}$

$$\begin{cases} \int_{\Omega} \rho f_s \varphi \, d\mathbf{x} &= - \int_{\Omega} \operatorname{div}(\vec{e}_s) \varphi \, d\mathbf{x} - \int_{\Omega} \sigma \varphi \, d\mathbf{x}, \\ \int_{\Omega} \vec{f}_s \cdot \vec{\varphi} \, d\mathbf{x} &= - \int_{\Omega} \overrightarrow{\operatorname{grad}}(e_s) \cdot \vec{\varphi} \, d\mathbf{x}, \\ \int_{\Omega} f_{\sigma} \varphi \, d\mathbf{x} &= \int_{\Omega} e_s \varphi \, d\mathbf{x}. \end{cases}$$

For instance, the control is the temperature $e_s = v_{\partial}$

- ② Apply Green's formula:

$$\begin{cases} \int_{\Omega} \rho f_s \varphi \, d\mathbf{x} &= - \int_{\Omega} \operatorname{div}(\vec{e}_s) \varphi \, d\mathbf{x} - \int_{\Omega} \sigma \varphi \, d\mathbf{x}, \\ \int_{\Omega} \vec{f}_s \cdot \vec{\varphi} \, d\mathbf{x} &= \int_{\Omega} e_s \operatorname{div}(\vec{\varphi}) \, d\mathbf{x} + \int_{\partial\Omega} v_{\partial} (\vec{\varphi} \cdot \vec{\mathbf{n}}) \, d\gamma \\ \int_{\Omega} f_{\sigma} \varphi \, d\mathbf{x} &= \int_{\Omega} e_s \varphi \, d\mathbf{x}. \end{cases}$$

Energy functional - Discretization 2/3 matrix form

The discrete system:

$$\begin{cases} M_\rho \underline{f}_s(t) &= \tilde{D} \underline{e}_s(t) - M \underline{e}_\sigma, \\ \vec{M} \underline{f}_s(t) &= -\tilde{D}^\top \underline{e}_s(t) + \tilde{B} \underline{v}_\partial(t), \\ M \underline{f}_\sigma(t) &= M \underline{e}_s(t) \\ M_\partial \underline{y}_\partial(t) &= B^\top \underline{e}_u(t), \end{cases}$$

$$\tilde{D} := -\int_\Omega \operatorname{div}(\vec{\Phi}) \Phi^\top \, d\mathbf{x} \in \mathbb{R}^{\tilde{N} \times N}, \quad \tilde{B} := \int_{\partial\Omega} (\vec{\Phi} \cdot \vec{\mathbf{n}}) \cdot \Psi^\top \, d\gamma \in \mathbb{R}^{\tilde{N} \times N_\partial}$$

Compact form:

$$\underbrace{\begin{pmatrix} M_\rho & 0 & 0 & 0 \\ 0 & \vec{M} & 0 & 0 \\ 0 & 0 & M & 0 \\ 0 & 0 & 0 & M_\partial \end{pmatrix}}_{\tilde{M}_d} \underbrace{\begin{pmatrix} \underline{f}_s(t) \\ \underline{f}_s(t) \\ \underline{f}_\sigma(t) \\ -\underline{y}_\partial(t) \end{pmatrix}}_{\vec{f}_d} = \underbrace{\begin{pmatrix} 0 & \tilde{D} & -M & 0 \\ -\tilde{D}^\top & 0 & 0 & \tilde{B} \\ M & 0 & 0 & 0 \\ 0 & -\tilde{B}^\top & 0 & 0 \end{pmatrix}}_{\tilde{J}_d} \underbrace{\begin{pmatrix} \underline{e}_s(t) \\ \underline{e}_s(t) \\ \underline{e}_\sigma(t) \\ \underline{v}_\partial(t) \end{pmatrix}}_{\vec{e}_d}$$

Energy functional - Discretization 3/3 structure

- **Structure-preservation:** $\vec{e}_d^\top \tilde{M}_d \vec{f}_d = 0$ (thanks to $\tilde{J}_d = -\tilde{J}_d^*$)
- **Discrete closure relation:**

- Dulong-Petit's law and Gibbs' relation:

$$C_V \rho \partial_t e_s = e_s f_s \implies (\text{Solve ODE})$$

- Fourier's law:

$$\int_{\Omega} e_s \vec{e}_s \cdot \vec{\varphi} \, d\mathbf{x} = \int_{\Omega} \vec{f}_s \cdot \bar{\lambda} \cdot \varphi \, d\mathbf{x} \implies (\text{1st non-linear closure eqn.}),$$

- Entropy closure relation:

$$\int_{\Omega} \vec{f}_s \cdot \vec{e}_s \varphi \, d\mathbf{x} = - \int_{\Omega} f_\sigma e_\sigma \varphi \, d\mathbf{x} \implies (\text{2nd non-linear closure eqn.})$$

- **Discrete power balance:**

$$d_t U_d(t) = \underline{v}_\partial^\top(t) M_\partial \underline{y}_\partial(t)$$

Energy functional - Simulation 2/2 time-space simulation

Energy functional - Simulation 2/2 time-space simulation

Conclusion

- The integration by parts of one of the weak-form equations naturally leads to skew-symmetric representation with the boundary input/output ports;
- 2D (or 3D) problems are straightforward to address;
- Interconnection structure and Constitutive relations are discretized separately;
- Same method can be used for other port-Hamiltonian systems (higher-order differential operators like Euler-Bernoulli beam, or Kirchhoff-Love plate equations, etc.);
- Space varying coefficients can be easily taken into account;
- Nonlinear equations: non-quadratic Hamiltonian and non-linear interconnection structure;
- Thermodynamically consistent potentials can be dealt with for the heat equation;
- PFEM can be easily implemented using available Finite Element software allowing for complex geometries.

Ongoing work and open questions

- Other (mixed) choices of input/output are possible;
- Ongoing convergence analysis;
- Numerical methods for DAEs;
- Multiphysics systems modelling: some useful 2D testcases (fluid-structure interaction (FSI), thermal-structure coupling, fluid-thermal coupling);
- Design and implementation of control laws.

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