Thermodynamic Foundation of Mathematical Systems Theory - 3rd TFMST 2019

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

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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**

Overview

Thermodynamical hypotheses 1/2 Notations

- Spatial domain and physical parameters:
  - $\Omega \subset \mathbb{R}^{n\geq 1}$, a bounded open connected set.
  - $\overrightarrow{\mathbf{n}}$, 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.
  - $\overrightarrow{\mathbf{J}}_Q$, the heat flux.
  - $\overrightarrow{\mathbf{J}}_S := \beta \overrightarrow{\mathbf{J}}_Q$, the entropy flux.
  - $C_V := \left(\frac{\mathrm{d}u}{\mathrm{d}T}\right)_V$, the isochoric heat capacity.

Thermodynamical hypotheses 2/2 hypotheses

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

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

- **Gibbs' relation**:

$$\mathrm{d}U = T\,\mathrm{d}S \quad \Longrightarrow \quad \partial_t u(t,\mathbf{x}) = T(t,\mathbf{x})\,\partial_t s(t,\mathbf{x}).$$

- **Entropy evolution**:

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

  with $\sigma(t,\mathbf{x}) := \overrightarrow{\mathbf{grad}}(\beta)\cdot\overrightarrow{\mathbf{J}}_Q$, the irreversible entropy production.
- **Fourier's law**:

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

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

Overview

Lyapunov functional - Modeling 1/3 quadratic Hamiltonian

Consider the **quadratic Hamiltonian**:

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

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.

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

Lyapunov functional - Modeling 2/3 port-Hamiltonian system

- Defining as *flows* and *efforts*:

$$\begin{aligned} f_u &:= \partial_t u, & e_u &:= \frac{u}{C_V} \\ \vec{f}_Q &:= -\overrightarrow{\textbf{grad}}\left(\frac{u}{C_V}\right), & \vec{e}_Q &:= \vec{\mathbf{J}}_Q \end{aligned}$$

- Port-Hamiltonian system:

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

- 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 $\vec{f}_Q = -\overrightarrow{\textbf{grad}}(T)$
  - Fourier's law $\implies$ $\vec{e}_Q = -\overline{\overline{\lambda}} \cdot \overrightarrow{\textbf{grad}}(T)$ $\implies$ $\vec{e}_Q = \overline{\overline{\lambda}} \cdot \vec{f}_Q$
- **Power balance**:

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

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

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

Lyapunov functional - Discretization 1/4 weak form

1. *Weak form*: Taking arbitrary test functions φ and $\overrightarrow{\varphi}$

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

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

2. *Apply Green's formula*:

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

Lyapunov functional - Discretization 2/4 approximation bases

- *Finite-dimensional* bases:

$$\mathcal{X} := \text{span}\{\Phi\} := \text{span}\{(\varphi^i)_{1\le i\le N}\},$$
$$\boldsymbol{\mathcal{X}} := \text{span}\{\overrightarrow{\boldsymbol{\Phi}}\} := \text{span}\{(\overrightarrow{\boldsymbol{\varphi}}^k)_{1\le k\le \overrightarrow{\boldsymbol{N}}}\},$$
$$\mathcal{X}_\partial := \text{span}\{\Psi\} := \text{span}\{(\psi_\partial^m)_{1\le m\le N_\partial}\},$$

- Approximation:

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

and similarly for the other variables.

Lyapunov functional - Discretization 3/4 matrix form

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

$$\begin{cases} M_\rho \underline{f_u}(t) &= D\, \underline{e_Q}(t) + B\, \underline{v_\partial(t)}, \\ \overrightarrow{\boldsymbol{M}}\, \underline{f_Q}(t) &= -D^\top\, \underline{e_u}(t), \\ M_\partial\, \underline{y_\partial(t)} &= B^\top\, \underline{e_u}(t), \end{cases}$$

with the following sparse matrices:

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

Compact form:

$$\underbrace{\begin{pmatrix} M_\rho & 0 & 0 \\ 0 & \overrightarrow{\boldsymbol{M}} & 0 \\ 0 & 0 & M_\partial \end{pmatrix}}_{\mathcal{M}_d} \underbrace{\begin{pmatrix} \underline{f_u}(t) \\ \underline{\overrightarrow{\boldsymbol{f}}_Q}(t) \\ -\underline{y_\partial}(t) \end{pmatrix}}_{\overrightarrow{\boldsymbol{f}}_d} = \underbrace{\begin{pmatrix} 0 & D & B \\ -D^\top & 0 & 0 \\ -B^\top & 0 & 0 \end{pmatrix}}_{\mathcal{J}_d} \underbrace{\begin{pmatrix} \underline{e_u}(t) \\ \underline{\overrightarrow{\boldsymbol{e}}_Q}(t) \\ \underline{v_\partial}(t) \end{pmatrix}}_{\overrightarrow{\boldsymbol{e}}_d}$$

Lyapunov functional - Discretization 4/4 structure

- **Structure-preservation**: $\overrightarrow{\boldsymbol{e}}_d^\top \mathcal{M}_d \overrightarrow{\boldsymbol{f}}_d = 0$ (thanks to $\mathcal{J}_d = -\mathcal{J}_d^*$)
- **Discrete closure relations**:
  - Dulong-Petit's law:

$$\int_\Omega \rho C_V \, \partial_t e_u \, \varphi \, \mathrm{d}\mathbf{x} = \int_\Omega \rho f_u \, \varphi \, \mathrm{d}\mathbf{x} \quad \Longrightarrow \quad M_{\rho C_V} \frac{d}{dt} \underline{e_u} = M_\rho \underline{f_u},$$

  - Fourier's law:

$$\int_\Omega \overrightarrow{\boldsymbol{e}}_Q \cdot \overrightarrow{\boldsymbol{\varphi}} \, \mathrm{d}\mathbf{x} = \int_\Omega (\overline{\overline{\lambda}} \cdot \overrightarrow{\boldsymbol{f}}_Q) \cdot \overrightarrow{\boldsymbol{\varphi}} \, \mathrm{d}\mathbf{x} \quad \Longrightarrow \quad \overrightarrow{\boldsymbol{M}} \underline{e_Q} = \overrightarrow{\boldsymbol{\Lambda}} \underline{f_Q}$$

- **Discrete Hamiltonian**:

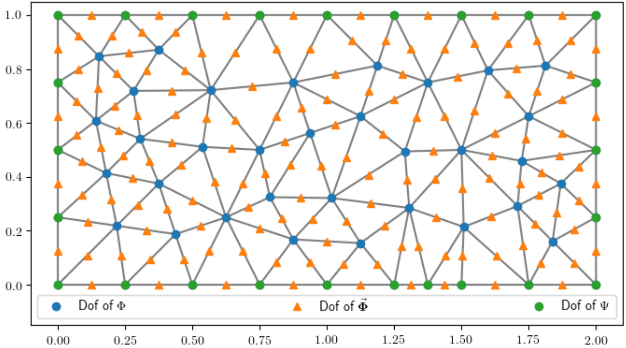
$$\mathcal{H}_d(t) = \frac{1}{2} \underline{e_u}^\top(t) \, M_{\rho C_V} \, \underline{e_u}(t)$$

- **Discrete power balance**:

$$d_t \mathcal{H}_d(t) = \underbrace{-\overrightarrow{\boldsymbol{f}}_Q^\top(t) \, \overrightarrow{\boldsymbol{\Lambda}} \, \overrightarrow{\boldsymbol{f}}_Q(t)}_{\text{discrete dissipation}} + \underbrace{\underline{v_\partial}^\top(t) \, M_\partial \, \underline{y_\partial}(t)}_{\text{discrete supplied power}}$$

Lyapunov functional - Simulation 1/2

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



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

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).

Overview

Entropy functional - Modeling 1/3 Hamiltonian Entropy

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

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

Choose u as *energy variable*, and compute the *co-energy variable* $\delta_u S = \frac{\mathrm{d}s}{\mathrm{d}u} = \beta$.

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

Entropy functional - Modeling 2/3 port-Hamiltonian system

- Defining as *flows* and *efforts*:

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

- Port-Hamiltonian system:

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

- 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: $u = \frac{C_V}{\beta} \quad \Longrightarrow \quad e_u = \frac{C_V}{u}$
  - Fourier's law: $\vec{e}_Q = \frac{1}{\beta^2} \overline{\overline{\lambda}} \cdot \overrightarrow{\textbf{grad}}(\beta) \quad \Longrightarrow \quad \vec{e}_Q = -\frac{1}{e_u^2} \overline{\overline{\lambda}} \cdot \vec{f}_Q$
- Power balance:

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

with the constitutive relations:

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

Entropy functional - Discretization 1/3 weak form

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

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

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

2. *Apply Green's formula*:

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

Entropy functional - Discretization 2/3 matrix form

The discrete system:

$$\left\{\begin{array}{ll} M_\rho \underline{f_u}(t) & = D\, \underline{e_Q}(t) + B\, \underline{v_\partial}(t), \\ \overrightarrow{M}\, \underline{f_Q}(t) & = -D^\top\, \underline{e_u}(t), \\ M_\partial\, \underline{y_\partial}(t) & = B^\top\, \underline{e_u}(t), \end{array}\right.$$

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

Compact form:

$$\underbrace{\begin{pmatrix} M_\rho & 0 & 0 \\ 0 & \overrightarrow{M} & 0 \\ 0 & 0 & M_\partial \end{pmatrix}}_{\mathcal{M}_d} \underbrace{\begin{pmatrix} \underline{f_u}(t) \\ \underline{f_Q}(t) \\ -\underline{y_\partial}(t) \end{pmatrix}}_{\overrightarrow{f}_d} = \underbrace{\begin{pmatrix} 0 & D & B \\ -D^\top & 0 & 0 \\ -B^\top & 0 & 0 \end{pmatrix}}_{\mathcal{J}_d} \underbrace{\begin{pmatrix} \underline{e_u}(t) \\ \underline{e_Q}(t) \\ \underline{v_\partial}(t) \end{pmatrix}}_{\overrightarrow{e}_d}$$

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:

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

  - Fourier's law:

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

- **Discrete power balance**:

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

Entropy functional - Simulation 1/

Overview

Energy functional - Modeling

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

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

Choosing s as *energy variable*, compute the *co-energy variable* $\delta_s U = \frac{\mathrm{d}u}{\mathrm{d}s} = T$.

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

Energy functional - Modeling 2/3 port-Hamiltonian system

- Defining as *flows* and *efforts*:

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

- Primary port-Hamiltonian system:

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

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

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

- Port-Hamiltonian system

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

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 $-\overrightarrow{\boldsymbol{e}}_S$ (*inward* entropy flux).
- Constitutive relations:
  - Dulong-Petit's law and Gibbs' relation:
    $C_V \rho \partial_t T = T \rho \partial_t s \quad \Longrightarrow \quad C_V \rho \partial_t e_s = e_s f_s$
  - Fourier's law: $e_s \overrightarrow{\boldsymbol{e}}_S = \overline{\overline{\lambda}} \cdot \overrightarrow{\boldsymbol{f}}_S$
  - Entropy closure relation: $\overrightarrow{\boldsymbol{f}}_S \cdot \overrightarrow{\boldsymbol{e}}_S + f_\sigma \, e_\sigma = 0$
- Power balance:

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

Entropy functional - Discretization 1/3 weak form

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

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

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

2. *Apply Green's formula*:

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

Energy functional - Discretization 2/3 matrix form

The discrete system:

$$\begin{cases} M_\rho \underline{f_s}(t) & = \tilde{D}\, \underline{e_S}(t) - M\, \underline{e_\sigma}, \\ \overrightarrow{\boldsymbol{M}}\, \underline{f_S}(t) & = -\tilde{D}^\top\, \underline{e_s}(t) + \tilde{B}\, \underline{v_\partial}(t), \\ M\, \underline{f_\sigma}(t) & = M\, \underline{e_s}(t) \\ M_\partial\, \underline{y_\partial}(t) & = B^\top\, \underline{e_u}(t), \end{cases}$$

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

Compact form:

$$\underbrace{\begin{pmatrix} M_\rho & 0 & 0 & 0 \\ 0 & \overrightarrow{\boldsymbol{M}} & 0 & 0 \\ 0 & 0 & M & 0 \\ 0 & 0 & 0 & M_\partial \end{pmatrix}}_{\tilde{\mathcal{M}}_d} \underbrace{\begin{pmatrix} \underline{f_s}(t) \\ \underline{f_S}(t) \\ \underline{f_\sigma}(t) \\ -\underline{y_\partial}(t) \end{pmatrix}}_{\overrightarrow{\boldsymbol{f}}_d} = \underbrace{\begin{pmatrix} 0 & \tilde{D} & -M & 0 \\ -\tilde{D}^\top & 0 & 0 & \tilde{B} \\ M & 0 & 0 & 0 \\ 0 & -\tilde{B}^\top & 0 & 0 \end{pmatrix}}_{\tilde{\mathcal{J}}_d} \underbrace{\begin{pmatrix} \underline{e_s}(t) \\ \underline{e_S}(t) \\ \underline{e_\sigma}(t) \\ \underline{v_\partial}(t) \end{pmatrix}}_{\overrightarrow{\boldsymbol{e}}_d}$$

Energy functional - Discretization 3/3 structure

- **Structure-preservation**: $\overrightarrow{\boldsymbol{e}}_d^\top \tilde{\mathcal{M}}_d \overrightarrow{\boldsymbol{f}}_d = 0$ (thanks to $\tilde{\mathcal{J}}_d = -\tilde{\mathcal{J}}_d^*$)
- **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:

$$\int_\Omega e_s \overrightarrow{\boldsymbol{e}}_S \cdot \overrightarrow{\boldsymbol{\varphi}} \, \mathrm{d}\mathbf{x} = \int_\Omega \overrightarrow{\boldsymbol{f}}_S \cdot \overline{\overline{\lambda}} \cdot \varphi \, \mathrm{d}\mathbf{x} \implies \text{(1st non-linear closure eqn.)},$$

  - Entropy closure relation:

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

- **Discrete power balance**:

$$d_t U_d(t) = v_\partial{}^\top(t) \, M_\partial \, y_\partial(t)$$

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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