Improving multiphysics simulation through port-Hamiltonian system theory

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28 June 2022

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Outline

Multiphysics problems

Port-Hamiltonian systems as a unified language for multiphysics

- Functional analytic structure
- The geometric definition

Mimetic discretization of port-Hamiltonian systems

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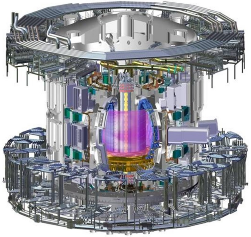
Challenges in muliphysics problems

Multiphysics problems are commonly found in industrial applications.

Aeroelasticity

Thermoelasticity



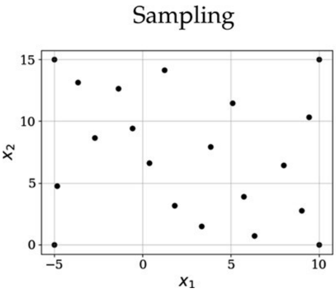
Magnetohydrodynamics

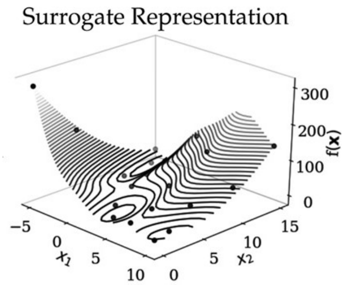
Challenges:

- Coupling between different models.
- Huge computational cost due to the large size of the models.
- Multidisciplinary optimization for dynamical systems.

Typical workflow in industry

- Specific modelling and numerical methods for each physical domain.
  - × The open character of systems is not properly considered.
  - × Numerical methods do not preserve the structure required to interconnect systems.
- Model reduction via statistical methods.
  - × The physical structure of the model is lost and first principles are violated.
  - × This methodology does not generalize to different problems.

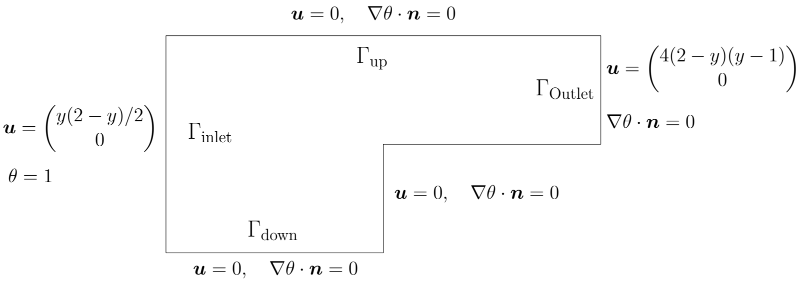




Example: convection dominated transport

Convection dominated transport of a passive scalar field in a Stokes flow[1]

$$
\begin{aligned}
\nu \Delta \boldsymbol{u} + \nabla p &= 0, & \boldsymbol{u} &: \text{Velocity},\\
\nabla \cdot \boldsymbol{u} &= 0, & p &: \text{Pressure},\\
-\varepsilon \Delta \theta + \boldsymbol{u} \cdot \nabla \theta &= 0. & \theta &: \text{Temperature}.
\end{aligned}
$$



Geometry and boundary conditions

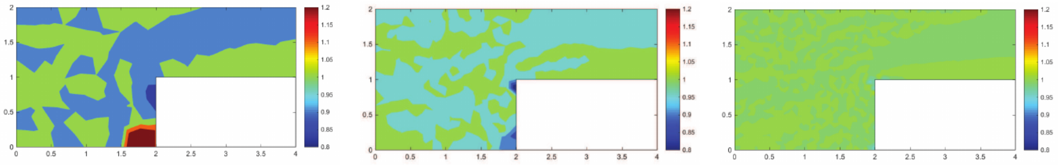
[1] Volker John et al. "On the Divergence Constraint in Mixed Finite Element Methods for Incompressible Flows". In: *SIAM Review* 59.3 (2017), pp. 492–544. DOI: 10.1137/15M1047696.

When multiphysics goes wrong

Exact solution for the temperature $\theta_{\text{ex}} = 1$.

- $(\boldsymbol{u}, p)$ discretized using the Taylor-Hood element $\mathbb{P}_2/\mathbb{P}_1$;
- θ discretized via Voronoi finite volume method.

The Taylor-Hood element does not lead to divergence free velocity $||\nabla \cdot \boldsymbol{u}||_{L^2(\Omega)} \neq 0$.



Refinement 1 | Refinement 2 | Refinement 3

Figure: Discrete temperature field θ obtained

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A unified language for multiphysics in engineering

The port-Hamiltonian paradigm provides a language to understand multiphysics:

- The idea of **interconnection** is formalized as **duality pairing**.
- **Physics** is at the core: port-Hamiltonian systems are **passive** with respect to the **energy storage function**.
- The **topological** and **metrical** structure of the equation is clearly separated (mimetic discretization).

A simple definition[2]

Definition (Port-Hamiltonian system)

Let $X_{\mathcal{S}}$, $X_{\mathcal{R}}$, $\mathcal{X}_S$ be Banach spaces. A port-Hamiltonian system is a triple $(\mathcal{D}, H, \mathcal{R})$:

- $\mathcal{D} \subset (X_{\mathcal{S}},\ X_{\mathcal{R}},\ X_{\mathcal{P}}) \times (X'_{\mathcal{S}},\ X'_{\mathcal{R}},\ X'_{\mathcal{P}})$ is a Dirac structure.
- $\mathcal{H} : U \to \mathbb{R}$ (with $U \subset X_{\mathcal{S}}$ open) is a Hamiltonian.
- $\mathcal{R} \subset X_{\mathcal{R}} \times X'_{\mathcal{R}}$ is a resistive relation.

The behavior of the pH system on an interval $\mathbb{I} \subset \mathbb{R}$ consists of all $(x, f_{\mathcal{R}}, f_{\mathcal{P}}, e_{\mathcal{R}}, e_{\mathcal{P}})$

- $x \in W^{1,2}_{\text{loc}}(\mathbb{I}, X_{\mathcal{S}})$, and $x(t) \in U$, $\forall t \in \mathbb{I}$,
- $(f_{\mathcal{R}}, e_{\mathcal{R}}) \in L^2_{\text{loc}}(\mathbb{I}; X_{\mathcal{R}} \times X'_{\mathcal{R}})$ and $(f_{\mathcal{P}}, e_{\mathcal{P}}) \in L^2_{\text{loc}}(\mathbb{I}; X_{\mathcal{P}} \times X'_{\mathcal{P}})$

that fulfill the differential inclusion

$$(-\frac{dx}{dt},\ f_{\mathcal{R}},\ f_{\mathcal{P}},\ D\mathcal{H}(x(t)),\ e_{\mathcal{R}},\ e_{\mathcal{P}}) \in \mathcal{D}, \qquad (f_{\mathcal{R}}, e_{\mathcal{R}}) \in \mathcal{R}, \qquad \text{for almost all } t \in \mathbb{I}.$$

[2] Timo Reis. “Some notes on port-Hamiltonian systems on Banach spaces”. In: *IFAC-PapersOnLine* 54.19 (2021). 7th IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control LHMNC 2021, pp. 223–229. DOI: 10.1016/j.ifacol.2021.11.082.

Some mathematical definitions

Dirac structure

Let X be a Banach space. A subspace $\mathcal{D} \subset X \times X^{'}$ is called a Dirac structure, if $\forall\, f \in X, e \in X^{'}$, it holds

$$(f, e) \in \mathcal{D} \iff \Big(\langle f \,|\hat{e}\rangle + \langle \hat{f} \,|e\rangle = 0, \quad \forall\, (\hat{f}, \hat{e}) \Big).$$

Hamiltonian

Let X be a Banach space and $U \subset X$ be open. A mapping $\mathcal{H} : U \to \mathbb{R}$ is a Hamiltonian if it is locally Lipschitz continuous and Gâteaux differentiable

Resistive relation

Let X be a Banach space. A relation $\mathcal{R} \subset X \times X^{'}$ is called resistive, if

$$\langle f \,|e\rangle \leq 0, \qquad \forall\, (f, e) \in \mathcal{R}.$$

Operators

If $J \in \mathcal{L}(X^{'}, X)$ is a skew-dual operator $\langle Jv \,| w\rangle = \langle v \,| -Jw\rangle \;\forall\, v, w \in X^{'}$ then $D = \{(Je, e) : e \in X^{'}\}$ is a Dirac structure[3].

If $R : X^{'} \to X$ is dissipative $\langle x' \,| G(x')\rangle \leq 0,\; \forall\, x' \in X^{'}$, then $\mathcal{R} = \{(G(e), e) : e \in X^{'}\}$ is a resistive relation.

$$\begin{pmatrix} \partial_t x \\ f_{\mathcal{R}} \\ f_{\mathcal{P}} \end{pmatrix} = J \begin{pmatrix} D\mathcal{H}(x(t)) \\ e_{\mathcal{R}} \\ e_{\mathcal{P}} \end{pmatrix}, \qquad f_{\mathcal{R}} = G(e_{\mathcal{R}}).$$

[3] T. Reis and T. Stykel. "Passivity, Port-Hamiltonian Formulation and Solution Estimates for a Coupled Magneto-Quasistatic System". In: *arXiv preprint arXiv:2205.15259* (2022).

Example: the wave equation

Consider the Hamiltonian

$$\mathcal{H} = (p,\, \kappa p)_{L^2(\Omega)} + (\boldsymbol{u},\, \rho^{-1}\boldsymbol{u})_{L^2(\Omega,\mathbb{R}^3)}.$$

where κ is the Bulk modulus and ρ is the density.

The wave equation on $\Omega \subset \mathbb{R}^3$ with Dirichlet boundary condition reads:

$$\begin{pmatrix} \partial_t p \\ \partial_t \boldsymbol{u} \end{pmatrix} = \begin{bmatrix} 0 & \mathrm{div} \\ \mathrm{grad}_w & 0 \end{bmatrix} \begin{pmatrix} D\mathcal{H}(p(t)) \\ D\mathcal{H}(\boldsymbol{u}(t)) \end{pmatrix}, \qquad D\mathcal{H}(p(t))|_{\partial\Omega} = g.$$

where grad_w corresponds to a weak definition of the gradient.
In this case: $X_{\mathcal{S}} = L^2(\Omega) \times H^{\mathrm{div}}(\Omega)'$, $X_{\mathcal{R}} = \emptyset$, $X_{\mathcal{P}} = H^{1/2}(\Omega)$ and

$$J = \begin{bmatrix} 0 & \mathrm{div} & \gamma_0 \\ \mathrm{grad}_w & 0 & 0 \\ \gamma_{\boldsymbol{n}} & 0 & 0 \end{bmatrix}$$

where γ_0 is the Dirichlet trace and $\gamma_{\boldsymbol{n}}$ is the normal trace.

Example: the Maxwell equations

Consider the Hamiltonian:

$$\mathcal{H} = \frac{1}{2}(\boldsymbol{D},\, \varepsilon^{-1}\boldsymbol{D})_{L^2(\Omega,\mathbb{R}^3)} + \frac{1}{2}(\boldsymbol{B},\, \mu^{-1}\boldsymbol{B})_{L^2(\Omega,\mathbb{R}^3)}.$$

where ε is the electric permittivity and μ is the magnetic permeability.

The Maxwell equation on $\Omega \subset \mathbb{R}^3$ with conducting boundary condition reads:

$$\frac{\partial}{\partial t}\begin{pmatrix}\boldsymbol{D}\\ \boldsymbol{B}\end{pmatrix} = \begin{bmatrix} 0 & \mathrm{curl} \\ -\,\mathrm{curl}_w & 0 \end{bmatrix}\begin{pmatrix} D\mathcal{H}(\boldsymbol{D}(t)) \\ D\mathcal{H}(\boldsymbol{B}(t))\end{pmatrix}, \qquad D\mathcal{H}(\boldsymbol{D}(t)) \times \boldsymbol{n}|_{\partial\Omega} = 0,$$

where curl_w corresponds to a weak curl operator and the field $\boldsymbol{D},\ \boldsymbol{B}$ satisfy

$$\nabla \cdot \boldsymbol{D} = 0, \qquad \nabla \cdot \boldsymbol{B} = 0.$$

In this case: $X_{\mathcal{S}} = L^2(\Omega,\mathbb{R}^3) \times H^{\mathrm{curl}}(\Omega, \mathrm{div} = 0)',\ X_{\mathcal{R}} = \emptyset,\ X_{\mathcal{P}} = \emptyset$ and

$$J = \begin{bmatrix} 0 & \mathrm{curl} \\ \mathrm{curl}_w & 0 \end{bmatrix}.$$

And many more

The same framework applies to

- Linear and non-linear solid mechanics (beams, plates, shells, etc.).
- Fluid dynamics.
- Chemical reactions.

Outline

The canonical geometric port-Hamiltonian system

Distributed port-Hamiltonian were initially defined in a differential geometric setting[4]. Given two fields of smooth differential forms $\alpha^p \in \Lambda^p(\Omega)$ and $\beta \in$

$$\begin{pmatrix} \partial_t \alpha^p \\ \partial_t \beta^q \end{pmatrix} = - \begin{bmatrix} 0 & (-1)^r \, \mathrm{d} \\ \mathrm{d} & 0 \end{bmatrix} \begin{pmatrix} \delta_\alpha H^{n-p} \\ \delta_\beta H^{n-q} \end{pmatrix}$$

[4] A.J. van der Schaft and B.M. Maschke. "Hamiltonian formulation of distributed-parameter systems with boundary energy flow". In: *Journal of Geometry and Physics* 42.1 (2002), pp. 166–194. DOI: 10.1016/S0393-0440(01)00083-3.

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Reis, Timo. "Some notes on port-Hamiltonian systems on Banach spaces". In: *IFAC-PapersOnLine* 54.19 (2021). 7th IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control LHMNC 2021, pp. 223–229. DOI: 10.1016/j.ifacol.2021.11.082.

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