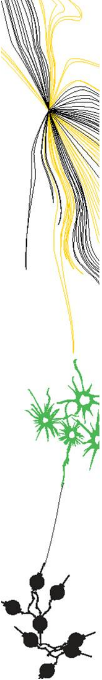

Improving multiphysics simulation through port-Hamiltonian system theory

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Outline

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Multiphysics problems

Port-Hamiltonian systems as a unified language for multiphysics

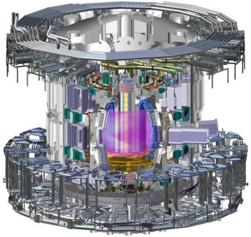
Mimetic discretization of port-Hamiltonian systems

Challenges in muliphysics problems

Multiphysics problems are commonly found in industrial applications.

Aeroelasticity

Thermoelasticity



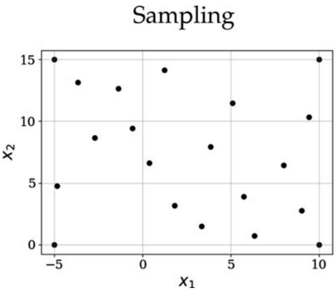
Magnetohydrodynamics

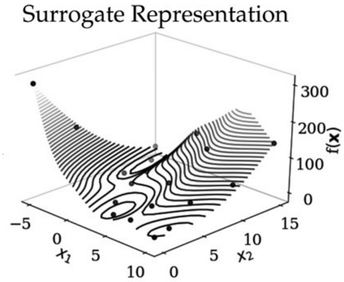
Challenges:

- 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.

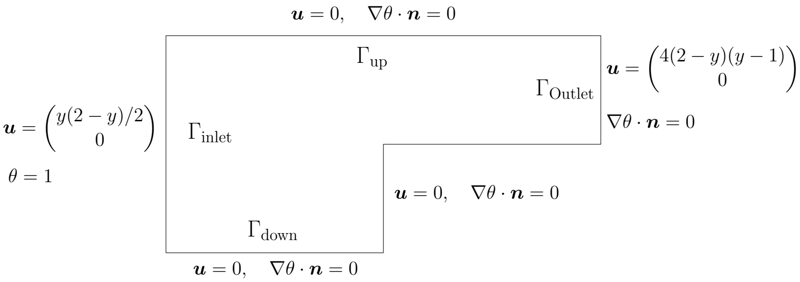




Example: convection dominated transport

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

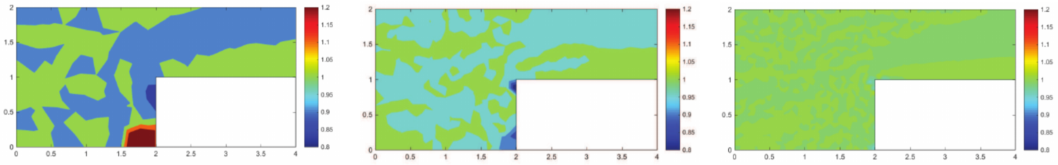
[1] Volker John et al. "On the Divergence Constraint in Mixed Finite Element Methods for Incompressible Flows". In: *SIAM Review* 59.3 (2017), pp. 492–544. DOI: 10.1137/15M1047696.

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

Outline

A unified language for multiphysics in engineering

The port-Hamiltonian (pH) 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).

Finite dimensional pH systems

Still not a well established theory

There is **not a unique definition** of pH systems, even in finite dimension.

Definition (Finite dimensional pH system)

The time-invariant dynamical system

$$\dot{\mathbf{x}} = (\mathbf{J} - \mathbf{R})\, \nabla H(\mathbf{x}) + \mathbf{B}\mathbf{u},$$
$$\mathbf{y} = \mathbf{B}^\top\, \nabla H(\mathbf{x}),$$

where $\mathbf{x}$ is the state, $\mathbf{u}$ the control input, $\mathbf{y}$ the collocated output and

- $H(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$, the Hamiltonian, is bounded from below.
- $\mathbf{J} = -\mathbf{J}^\top$ the interconnection operator.
- $\mathbf{R} = \mathbf{R}^\top \in \mathbb{R}^{n\times n}$, $\mathbf{R} \geq 0$ the resistive operator.
- $\mathbf{B} \in \mathbb{R}^{n\times m}$ the control operator.

is a pH system.

The geometric structure of pH systems[2]

Definition (Finite dimensional Dirac structure)

Given a finite-dimensional vector space F and its dual $E = F'$ with respect to the duality product $\langle \cdot \,|\cdot \rangle : E \times F \to \mathbb{R}$, consider the symmetric bilinear form:

$$\langle\langle\, (\mathbf{f}_1, \mathbf{e}_1), (\mathbf{f}_2, \mathbf{e}_2)\,\rangle\rangle := \langle \mathbf{e}_1 \,|\mathbf{f}_2 \rangle + \langle \mathbf{e}_2 \,|\mathbf{f}_1 \rangle, \;\text{ where } (\mathbf{f}_i, \mathbf{e}_i) \in B, \; i = 1, 2.$$

A Dirac structure on $B := F \times E$ is a linear subspace $D \subset B$ which equals its orthogonal companion with respect to $\langle\langle \cdot, \cdot \rangle\rangle$, *i.e.* $D = D^{[\perp]}$, where:

$$D^{[\perp]} := \left\{ (\mathbf{f}, \mathbf{e}) \in B \;\mid\; \langle\langle\, (\mathbf{f}, \mathbf{e}), (\widehat{\mathbf{f}}, \widehat{\mathbf{e}})\,\rangle\rangle = 0, \; \forall \; (\widehat{\mathbf{f}}, \widehat{\mathbf{e}}) \in D \right\}.$$

Theorem

Given a finite-dimensional vector space F and its dual $E = F'$ a subspace $D \subset F \times E$ is a Dirac structure iff $\langle \mathbf{e} \,|\mathbf{f} \rangle = 0$ and $\dim D = \dim F$.

[2] T. J. Courant. "Dirac manifolds". In: *Transactions of the American Mathematical Society* 319.2 (1990), pp. 631–661. ISSN: 0002-9947. DOI: 10.2307/2001258.

Dirac structure and pH systems

From classical matrix factorization $\exists\, \mathbf{G} \in \mathbb{R}^{k\times n}$ and $\mathbf{K} = \mathbf{K}^\top \in \mathbb{R}^{k\times k}$, $\mathbf{K} \geq 0$ such that $\mathbf{R} = \mathbf{G}^\top\, \mathbf{K}\mathbf{G}$.

Dirac structure representation

Considering the following **ports**:

- the **storage ports** $(\mathbf{f}_x, \mathbf{e}_x) := (-\dot{\mathbf{x}}, \nabla H(\mathbf{x})) \in \mathbb{R}^n \times \mathbb{R}^n$;
- the **resistive ports** $(\mathbf{f}_r, \mathbf{e}_r) \in \mathbb{R}^k \times \mathbb{R}^k$;
- the **interconnection ports** $(\mathbf{f}_u, \mathbf{e}_u) := (\mathbf{y}, \mathbf{u}) \in \mathbb{R}^m \times \mathbb{R}^m$.

Given this port behavior, the pH system rewrites

$$\begin{pmatrix} \mathbf{f}_x \\ \mathbf{f}_r \\ \mathbf{f}_u \end{pmatrix} = \underbrace{\begin{bmatrix} -\mathbf{J} & \mathbf{G}^\top & -\mathbf{B} \\ \mathbf{G} & \mathbf{0} & \mathbf{0} \\ \mathbf{B}^\top & \mathbf{0} & \mathbf{0} \end{bmatrix}}_{\mathbf{J}_e} \begin{pmatrix} \mathbf{e}_x \\ \mathbf{e}_r \\ \mathbf{e}_u \end{pmatrix}, \qquad \mathbf{e}_r = \mathbf{K}\mathbf{f}_r.$$

Since $\mathbf{J}_e$ is skewsymmetric its graph defines a Dirac structure.

A simple definition[3]

Definition (Port-Hamiltonian system)

Let $X_{\mathcal{S}},\ X_{\mathcal{R}},\ X_{\mathcal{S}}$ 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 $(x, f_{\mathcal{R}}, f_{\mathcal{P}}, e_{\mathcal{R}}, e_{\mathcal{P}})$

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

that fulfill the differential inclusion

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

[3] 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

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

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

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

Operators

If $J \in \mathcal{L}(X^{'}, X)$ is a skew-dual operator $\langle w \,|\, Jv\rangle = \langle v \,|\, -Jw\rangle \; \forall \, v, w \in X^{'}$ then $D = \{(Je, e) : e \in X^{'}\}$ is a Dirac structure[4].

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

$$\begin{pmatrix} -\partial_t x \\ f_{\mathcal{R}} \\ f_{\mathcal{P}} \end{pmatrix} = J \begin{pmatrix} D_x \mathcal{H} \\ e_{\mathcal{R}} \\ e_{\mathcal{P}} \end{pmatrix}, \qquad e_{\mathcal{R}} = K(f_{\mathcal{R}}).$$

[4] 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

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

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:

$$\frac{\partial}{\partial t}\begin{pmatrix} p \\ \boldsymbol{v} \end{pmatrix} = \begin{bmatrix} 0 & \mathrm{div} \\ \mathrm{grad}_w & 0 \end{bmatrix}\begin{pmatrix} D_p\mathcal{H} \\ D_{\boldsymbol{v}}\mathcal{H} \end{pmatrix}, \qquad \gamma_0(D_p\mathcal{H}) = u \in H^{1/2}(\partial\Omega),$$

where grad_w corresponds to a weak gradient and γ_0 is the Dirichlet trace.
In this case: $X_{\mathcal{S}} = L^2(\Omega) \times H^{\mathrm{div}}(\Omega)',\ X_{\mathcal{R}} = \emptyset,\ X_{\mathcal{P}} = H^{-1/2}(\partial\Omega)$ and

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

where $\gamma_{\boldsymbol{n}}$ 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:

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

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: $X_{\mathcal{S}} = L^2(\Omega,\mathbb{R}^3|\,\mathrm{div}=0)\times H_0^{\mathrm{curl}}(\Omega|\,\mathrm{div}=0)',\ X_{\mathcal{R}} = \emptyset,\ X_{\mathcal{P}} = \emptyset$ 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[5].
In this setting the duality is the Hodge duality, given by the Hodge star $\star$.
Given two fields of smooth differential forms $\alpha^p \in \Lambda^p(\Omega)$ and $\beta \in \Lambda^q(\Omega)$ the following systems

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

together will appropriate boundary conditions are port-Hamiltonian distributed systems.

[5] 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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Bibliography I

- Courant, T. J. "Dirac manifolds". In: *Transactions of the American Mathematical Society* 319.2 (1990), pp. 631–661. ISSN: 0002-9947. DOI: 10.2307/2001258.
- John, Volker 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.
- Reis, T. and T. Stykel. "Passivity, Port-Hamiltonian Formulation and Solution Estimates for a Coupled Magneto-Quasistatic System". In: *arXiv preprint arXiv:2205.15259* (2022).
- 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.
- Schaft, A. van der and D. Jeltsema. "Port-Hamiltonian Systems Theory: An Introductory Overview". In: *Foundations and Trends® in Systems and Control* 1.2–3 (2014), pp. 173–378.

Bibliography II

van der Schaft, A.J. 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.