

Improving multiphysics simulation through port-Hamiltonian system theory

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Outline

Multiphysics problems

Port-Hamiltonian systems as a unified language for multiphysics

- Functional analytic structure

- The geometric formulation

Mimetic discretization of port-Hamiltonian systems

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Challenges in multiphysics problems

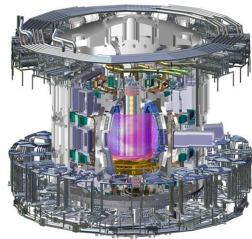
Multiphysics problems are commonly found in industrial applications.



Aeroelasticity



Thermoelasticity



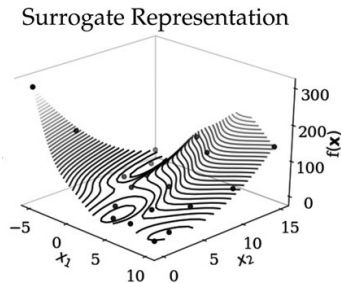
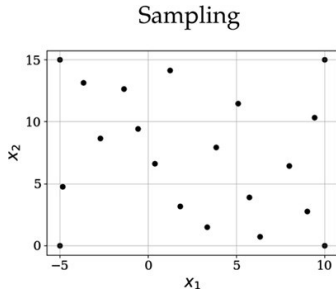
Magnetohydrodynamics

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

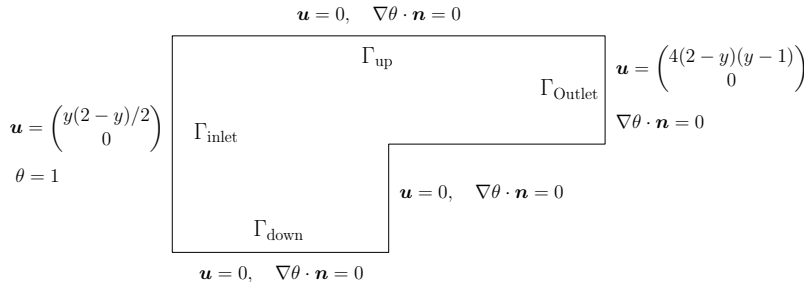
- ▶ **Specific modelling** and numerical methods for each physical domain.
 - The **open character** of systems is **not considered**.
 - Numerical methods do not preserve the structure required to interconnect systems.
- ▶ Model reduction via statistical methods.
 - The **physical structure is lost** 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 flow¹

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



Geometry and boundary conditions

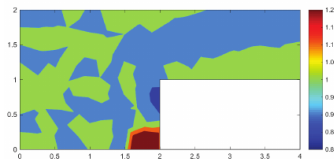
¹Volker John et al. "On the Divergence Constraint in Mixed Finite Element Methods for Incompressible Flows". In: *SIAM Review* 59.3 (2017), pp. 492–544. DOI: 10.1137/15M1047696.

When multiphysics goes wrong

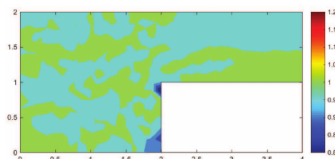
Exact solution for the temperature $\theta_{\text{ex}} = 1$.

- ▶ (\mathbf{u}_h, p_h) represented using the Taylor-Hood element $\mathbb{P}_2/\mathbb{P}_1$;
- ▶ θ_h obtained via Voronoi finite volume method.

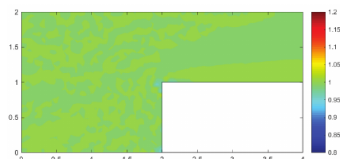
The Taylor-Hood element does not lead to divergence free velocity $\|\nabla \cdot \mathbf{u}_h\|_{L^2(\Omega)} \neq 0$.



Refinement 1



Refinement 2



Refinement 3

Figure: Discrete temperature field θ_h obtained

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A unified language for multiphysics in engineering

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

- ▶ **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).
- ▶ PH systems are **closed under interconnection**.



A quest for duality

The concept of **interconnection** and the port behavior of pH systems is mathematically formalized as **duality pairing**. How exactly is that defined ?

Finite dimensional pH systems

A theory still under developement

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

Definition (Finite dimensional pH system)

The time-invariant dynamical system

$$\begin{aligned}\dot{\mathbf{x}} &= (\mathbf{J} - \mathbf{R}) \nabla_{\mathbf{x}} H + \mathbf{B} \mathbf{u}, \\ \mathbf{y} &= \mathbf{B}^{\top} \nabla_{\mathbf{x}} H,\end{aligned}$$

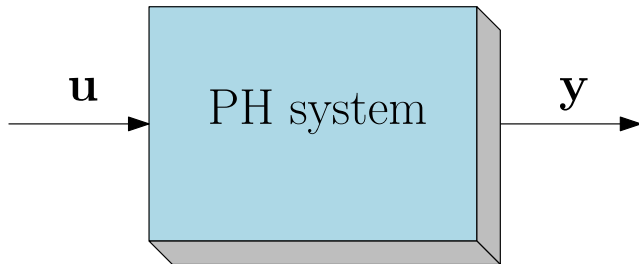
where \mathbf{x} is the state, \mathbf{u} the control input, \mathbf{y} the collocated output and

- ▶ $H(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$, 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.

Finite dimensional pH systems

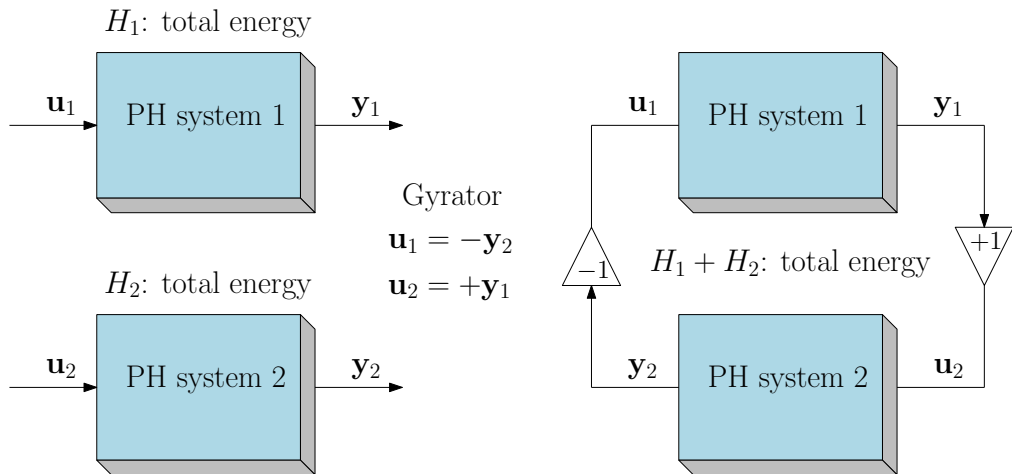
H : total energy



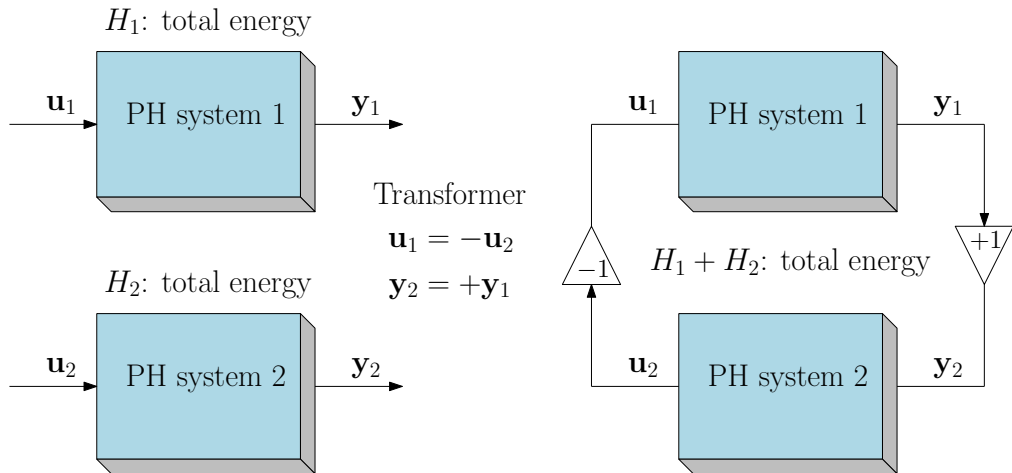
Lossless ($\mathbf{R} = \mathbf{0}$): $\dot{H} = \mathbf{u}^\top \mathbf{y}$

Passive: $\dot{H} \leq \mathbf{u}^\top \mathbf{y}$

Energy preserving interconnection of pHs



Energy preserving interconnection of pHs



The geometric structure of pH systems²

Definition (Dirac structure)

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

$$\langle\langle (f_1, e_1), (f_2, e_2) \rangle\rangle := \langle e_1 | f_2 \rangle + \langle e_2 | f_1 \rangle, \quad (f_i, e_i) \in B = F \times E, \quad i = 1, 2.$$

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

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

Theorem (Finite dimensional Dirac structure)

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

²T. 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 **port behavior**:

- ▶ the **storage ports** $(\mathbf{f}_x, \mathbf{e}_x) := (-\dot{\mathbf{x}}, \nabla_{\mathbf{x}} H) \in \mathbb{R}^n \times \mathbb{R}^n$;
- ▶ 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

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

Since \mathbf{J}_e is skewsymmetric its graph $\{(\mathbf{f}, \mathbf{e}) \in F \mid \mathbf{f} = \mathbf{J}_e \mathbf{e}\}$ is a Dirac structure.

A simple definition³

Definition (Port-Hamiltonian system)

Let X_S , X_R , X_P be Banach spaces. A port-Hamiltonian system is a triple $(\mathcal{D}, H, \mathcal{R})$:

- ▶ $\mathcal{D} \subset (X_S, X_R, X_P) \times (X'_S, X'_R, X'_P)$ is a Dirac structure.
- ▶ $H : U \rightarrow \mathbb{R}$ (with $U \subset X_S$ open) is a Hamiltonian.
- ▶ $\mathcal{R} \subset X_R \times X'_R$ is a resistive relation.

The behavior of the pH system on an interval $\mathbb{I} \subset \mathbb{R}$ consists of all (x, f_R, f_P, e_R, e_P)

- ▶ $x \in W_{\text{loc}}^{1,2}(\mathbb{I}, X_S)$, and $x(t) \in U$, $\forall t \in \mathbb{I}$,
- ▶ $(f_R, e_R) \in L_{\text{loc}}^2(\mathbb{I}; X_R \times X'_R)$ and $(f_P, e_P) \in L_{\text{loc}}^2(\mathbb{I}; X_P \times X'_P)$

that fulfill the differential inclusion

$$(-\partial_t x, f_R, f_P, D_x H, e_R, e_P) \in \mathcal{D}, \quad (f_R, e_R) \in \mathcal{R}, \quad \text{for almost all } t \in \mathbb{I}.$$

³Timo 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.

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

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

Hamiltonian

Let X be a Banach space and $U \subset X$ be open. A mapping $H : U \rightarrow \mathbb{R}$ 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

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

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 $\mathcal{D} = \{(Je, e) : e \in X'\}$ is a Dirac structure⁴.

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

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

⁴T. 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

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

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

The wave equation on \mathbb{R}^3 with distributed input

$$\frac{\partial}{\partial t} \begin{pmatrix} p \\ \mathbf{v} \end{pmatrix} = \begin{bmatrix} 0 & \operatorname{div} \\ \operatorname{grad}_w & 0 \end{bmatrix} \begin{pmatrix} D_p H \\ D_{\mathbf{v}} H \end{pmatrix} + \begin{bmatrix} \operatorname{Id} \\ 0 \end{bmatrix} u, \quad \operatorname{grad}_w \text{ is the weak gradient,}$$

$$y = \begin{bmatrix} \operatorname{Id} & 0 \end{bmatrix} \begin{pmatrix} D_p H \\ D_{\mathbf{v}} H \end{pmatrix},$$

Spaces: $X_{\mathcal{S}} = L^2(\mathbb{R}^3) \times H^{\operatorname{div}}(\mathbb{R}^3)'$, $X_{\mathcal{R}} = \emptyset$, $X_{\mathcal{P}} = L^2(\mathbb{R}^3)$.

$$J = \begin{bmatrix} 0 & -\operatorname{div} & -\operatorname{Id} \\ -\operatorname{grad}_w & 0 & 0 \\ \operatorname{Id} & 0 & 0 \end{bmatrix}.$$

Example: the Maxwell equations

Consider the Hamiltonian:

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

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

$$\frac{\partial}{\partial t} \begin{pmatrix} \mathbf{D} \\ \mathbf{B} \end{pmatrix} = \begin{bmatrix} 0 & \text{curl}_w \\ -\text{curl} & 0 \end{bmatrix} \begin{pmatrix} D_{\mathbf{D}}H \\ D_{\mathbf{B}}H \end{pmatrix}, \quad \begin{aligned} \nabla \cdot \mathbf{D} &= 0, & \nabla \cdot \mathbf{B} &= 0, \\ D_{\mathbf{D}}H \times \mathbf{n}|_{\partial\Omega} &= \mathbf{E} \times \mathbf{n}|_{\partial\Omega} = 0, \end{aligned}$$

where curl_w corresponds to a weak curl operator

Spaces: $H_0^{\text{curl}}(\Omega | \text{div} = 0)' \times X_{\mathcal{S}} = L^2(\Omega; \mathbb{R}^3 | \text{div} = 0)$, $X_{\mathcal{R}} = \emptyset$, $X_{\mathcal{P}} = \emptyset$.

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

And many more

The same framework applies to

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

However some aspects need further clarification:

- ▶ how to describe generic boundary conditions?
- ▶ how to represent the duality in a discrete setting?

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Functional analytic structure

The geometric formulation

Mimetic discretization of port-Hamiltonian systems

Geometric Dirac structure⁵

Dirac structure for differential forms

On a Riemannian oriented manifold Ω consider

- ▶ the flows $(f_1^p, f_2^q, f_{\partial}^{n-p}) \in F = \Lambda^p(\Omega) \times \Lambda^q(\Omega) \times \Lambda^{n-p}(\partial\Omega)$,
- ▶ the efforts $(e_1^{n-p}, e_2^{n-q}, e_{\partial}^{n-q}) \in E = \Lambda^{n-p}(\Omega) \times \Lambda^{n-q}(\Omega) \times \Lambda^{n-q}(\partial\Omega)$,

with $p + q = n + 1$ and $\Lambda^k(\Omega)$ is the space of smooth k -forms.

The following subset $\mathcal{D} \subset F \times E$ defines a Dirac structure

$$\begin{pmatrix} f_1^p \\ f_2^q \end{pmatrix} = \begin{bmatrix} 0 & (-1)^{pq+1} d \\ d & 0 \end{bmatrix} \begin{pmatrix} e_1^{n-p} \\ e_2^{n-q} \end{pmatrix}, \quad \begin{pmatrix} f_{\partial}^{n-p} \\ e_{\partial}^{n-q} \end{pmatrix} = \begin{bmatrix} \text{tr} & 0 \\ 0 & (-1)^p \text{tr} \end{bmatrix} \begin{pmatrix} e_1^{n-p} \\ e_2^{n-q} \end{pmatrix}.$$

The key is that this subset verify the following power balance (Stokes formula)

$$\langle e_1^{n-p} | f_1^p \rangle_{\Omega} + \langle e_2^{n-q} | f_2^q \rangle_{\Omega} + \langle e_{\partial}^{n-q} | f_{\partial}^{n-p} \rangle_{\partial\Omega} = 0.$$

⁵A.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.

Hyperbolic dynamical systems

Consider the following dynamical system with boundary input and observation

$$\begin{pmatrix} \partial_t \alpha^p \\ \partial_t \beta^q \end{pmatrix} = - \begin{bmatrix} 0 & (-1)^{pq+1} \mathbf{d} \\ \mathbf{d} & 0 \end{bmatrix} \begin{pmatrix} \delta_\alpha H^{n-p} \\ \delta_\beta H^{n-q} \end{pmatrix}, \quad (-1)^p \operatorname{tr} \delta_\beta H^{n-q} = u^{n-q},$$
$$y^{n-p} = \operatorname{tr} \delta_\alpha H^{n-p},$$

where the variational derivative is defined by

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} H(\mu^k + \varepsilon \delta \mu^k) = \langle \delta_\mu H^{n-p} | \delta \mu^k \rangle_\Omega,$$

Considering the following **port behavior**:

- ▶ the **storage ports** $(f_1^p, f_2^q, e_1^{n-p}, e_2^{n-q}) := (-\partial_t \alpha^p, -\partial_t \beta^q, \delta_\alpha H^{n-p}, \delta_\beta H^{n-q})$;
- ▶ the **interconnection ports** $(f_\partial^{n-p}, e_\partial^{n-q}) := (y^{n-p}, u^{n-q})$.

Then the dynamical system defines a Dirac structure.

The geometric wave and Maxwell equations

Assume $\Omega \subset \mathbb{R}^3$.

Case $p = 3, q = 1$ Wave equation.

$$\begin{pmatrix} \partial_t p^3 \\ \partial_t \mathbf{u}^1 \end{pmatrix} = - \begin{bmatrix} 0 & \operatorname{div} \\ \operatorname{grad} & 0 \end{bmatrix} \begin{pmatrix} \delta_p H^0 \\ \delta_{\mathbf{u}} H^2 \end{pmatrix}, \quad -\delta_{\mathbf{u}} H^2 \cdot \mathbf{n}|_{\partial\Omega} = u^2, \\ y^0 = \delta_p H^0|_{\partial\Omega}.$$

Case $p = 2, q = 2$ Maxwell equation

$$\begin{pmatrix} \partial_t \mathbf{D}^2 \\ \partial_t \mathbf{B}^2 \end{pmatrix} = \begin{bmatrix} 0 & \operatorname{curl} \\ -\operatorname{curl} & 0 \end{bmatrix} \begin{pmatrix} \delta_{\mathbf{D}} H^1 \\ \delta_{\mathbf{B}} H^1 \end{pmatrix}, \quad \mathbf{n} \times (\delta_{\mathbf{B}} H^1 \times \mathbf{n})|_{\partial\Omega} = u^1, \\ y^1 = \delta_{\mathbf{D}} H^1 \times \mathbf{n}|_{\partial\Omega}.$$

What about the functional analytic structure?

Consider the Sobolev space

$$H\Lambda^k(\Omega) := \{\mu^k \in L^2\Lambda^k(\Omega) \mid d\mu^k \in L^2\Omega^{k+1}(\Omega)\}, \quad k = 0, \dots, n-1.$$

One could replace spaces of smooth forms with forms living in this Sobolev space. However, the **Stokes formula** has only been proven when **more regularity** is present.

*Theorem (Theorem 6.3 in D. Arnold *Finite Element Exterior calculus*)*

In a manifold Ω with Lipschitz boundary it holds

$$\int_{\Omega} d\mu \wedge \lambda + (-1)^k \int_{\Omega} \alpha \wedge d\beta = \int_{\partial\Omega} \text{tr } \mu \wedge \text{tr } \lambda, \quad \mu \in H^1\Lambda^k(\Omega), \quad \lambda \in H\Lambda^{n-k-1}(\Omega),$$

where $H^1\Lambda^k(\Omega)$ is the space of k -forms with coefficient in $H^1(\Omega)$.

Nevertheless, using conforming finite elements for $H\Lambda^k$, one can obtain a discrete version of the Dirac structure.

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The adjoint pH structure

Using the **Hodge isomorphism**, an adjoint pH structure (associated to an adjoint Dirac structure) is computed

Adjoint pH system

$$\begin{pmatrix} \partial_t \alpha^{n-p} \\ \partial_t \beta^{n-q} \end{pmatrix} = - \begin{bmatrix} 0 & (-1)^{a_0} d^* \\ (-1)^{a_1} d^* & 0 \end{bmatrix} \begin{pmatrix} \delta_\alpha \hat{H}^p \\ \delta_\beta \hat{H}^q \end{pmatrix}, \quad (-1)^{a_3} \operatorname{tr} \star \delta_\beta \hat{H}^q = u^{n-q},$$
$$y^{n-p} = \operatorname{tr} \star \delta_\alpha \hat{H}^p,$$






where d^* is the codifferential and a_i are coefficients due to the Hodge star.

Mimetic dual-field discretization⁶


- ▶ Combining the port-Hamiltonian system and its adjoint, **two dynamical systems**, whose dynamics is **ruled by skew-adjoint operators** are constructed.
- ▶ The two systems are put into **weak form** considering variables that live in $H\Lambda^k(\Omega)$ using the L^2 inner product. The codifferential is interpreted weakly using the integration by parts formula.
- ▶ Conforming finite element $\mathcal{V}^k \subset H\Lambda^k(\Omega)$ are used for the variables.

⁶Yi Zhang et al. “A mass-, kinetic energy- and helicity-conserving mimetic dual-field discretization for three-dimensional incompressible Navier-Stokes equations, part I: Periodic domains”. In: *Journal of Computational Physics* (2021). DOI: [10.1016/j.jcp.2021.110868](https://doi.org/10.1016/j.jcp.2021.110868).

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