On the discrete equivalence of Lagrangian, Hamiltonian and mixed finite element formulations for linear wave phenomena

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Summary

A matter of representation: equivalent formulations for wave equations

Discrete equivalence of Lagrangian and Hamiltonian forms

Equivalence of Lagrangian and port-Hamiltonian discrete systems

Outline

A matter of representation: equivalent formulations for wave equations

Discrete equivalence of Lagrangian and Hamiltonian forms

Equivalence of Lagrangian and port-Hamiltonian discrete systems

When are two things equivalent?

Arena

Colosseum

The Arena is a smaller version of the Colosseum,

When are two things equivalent?

Arena

Colosseum

and still hosts concerts and lyrical spectacles.

Equivalent representation of mechanics: the wave equation

$$\rho\partial_{tt}q = \nabla\cdot(k\nabla q), \qquad \nabla q\cdot\boldsymbol{n}|_{\partial\Omega} = 0.$$

The total energy comprises the kinetic end potential energy

$$T(q) = \frac{1}{2}\int_\Omega \rho\dot{q}^2\mathrm{d}\Omega, \qquad U(q) = \frac{1}{2}\int_\Omega k||\nabla q||^2\mathrm{d}\Omega.$$

Different visions of the same equation

- **Lagrangian formalism**: the motion minimizes

$$S(q) = \int_{t_1}^{t_2} L\mathrm{d}t, \qquad L(q) = T(q) - U(q).$$

- **Hamiltonian formalism**: the motion minimizes

$$S(q,p) = \int_{t_1}^{t_2} (p\dot{q} - H)\mathrm{d}t, \qquad H(q,p) = T(p) + U(q).$$

The Hamiltonian is the Legendre transform of the Lagrangian

Variational characterization

Euler Lagrange equations

The minimization of $S(q)$ leads to Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta L}{\delta \dot{q}} - \frac{\delta L}{\delta q} = 0, \qquad \frac{\delta L}{\delta \dot{q}} = \rho \dot{q}, \quad \frac{\delta L}{\delta q} = -\nabla \cdot (k \nabla q).$$

Hamilton's equations

The minimization of $S(q, p)$ leads to Hamilton's equations

$$\begin{bmatrix} \dot{p} \\ \dot{q} \end{bmatrix} = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix} \begin{bmatrix} \delta_p H \\ \delta_q H \end{bmatrix}, \qquad \begin{aligned} \delta_p H &= p/\rho, \\ \delta_q H &= -\nabla \cdot (k \nabla q). \end{aligned}$$

Equivalent representation of mechanics: the Maxwell equations

$$\varepsilon \ddot{\boldsymbol{A}} = -\nabla \times (\mu^{-1} \nabla \times \boldsymbol{A}), \qquad (\nabla \times \boldsymbol{A}) \times \boldsymbol{n}|_{\partial\Omega} = 0.$$

The total energy comprises the electric end magnetic energy

$$T(\boldsymbol{A}) = \frac{1}{2} \int_{\Omega} \varepsilon ||\dot{\boldsymbol{A}}||^2 \mathrm{d}\Omega, \qquad U(\boldsymbol{A}) = \frac{1}{2} \int_{\Omega} \mu^{-1} ||\nabla \times \boldsymbol{A}||^2 \mathrm{d}\Omega,$$

where $\boldsymbol{A}$ is the magnetic potential, satisfying $\dot{\boldsymbol{A}} = -\boldsymbol{E}$.

Different visions of the same equation

- **Lagrangian formalism**: the motion minimizes

$$S(\boldsymbol{A}) = \int_{t_1}^{t_2} L \mathrm{d}t, \qquad L(\boldsymbol{A}) = T(\boldsymbol{A}) - U(\boldsymbol{A}).$$

- **Hamiltonian formalism**: the motion minimizes ($\boldsymbol{Y} = \varepsilon \dot{\boldsymbol{A}}$)

$$S(\boldsymbol{A}, \boldsymbol{Y}) = \int_{t_1}^{t_2} (\boldsymbol{Y} \cdot \dot{\boldsymbol{A}} - H) \mathrm{d}t, \qquad H(\boldsymbol{A}, \boldsymbol{Y}) = T(\boldsymbol{Y}) + U(\boldsymbol{A}).$$

Variational characterization

Euler Lagrange equations

The minimization of $S(\boldsymbol{A})$ leads to Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\delta L}{\delta \dot{\boldsymbol{A}}} - \frac{\delta L}{\delta \boldsymbol{A}} = 0, \qquad \frac{\delta L}{\delta \dot{\boldsymbol{A}}} = \varepsilon \dot{\boldsymbol{A}}, \quad \frac{\delta L}{\delta \boldsymbol{A}} = \nabla \times (\mu^{-1} \nabla \times \boldsymbol{A}).$$

Hamilton's equations

The minimization of $S(\boldsymbol{A}, \boldsymbol{Y})$ leads to Hamilton's equations

$$\begin{bmatrix} \dot{\boldsymbol{Y}} \\ \dot{\boldsymbol{A}} \end{bmatrix} = \begin{bmatrix} 0 & -\boldsymbol{I} \\ \boldsymbol{I} & 0 \end{bmatrix} \begin{bmatrix} \delta_{\boldsymbol{Y}} H \\ \delta_{\boldsymbol{A}} H \end{bmatrix}, \qquad \begin{aligned} \delta_{\boldsymbol{Y}} H &= \dot{\boldsymbol{A}}, \\ \delta_{\boldsymbol{A}} H &= \nabla \times (\mu^{-1} \nabla \times \boldsymbol{A}). \end{aligned}$$

Port-Hamiltonian derivation

The derivation of the equations of motion in port-Hamiltonian can be achieved via Hamiltonian reduction[1].
Writing the **wave equation** using the **velocity and stress** field, one obtains

$$\begin{bmatrix} \rho & 0 \\ 0 & c \end{bmatrix} \begin{bmatrix} \dot{v} \\ \dot{\boldsymbol{\sigma}} \end{bmatrix} = \begin{bmatrix} 0 & \nabla\cdot \\ \nabla & 0 \end{bmatrix} \begin{bmatrix} v \\ \boldsymbol{\sigma} \end{bmatrix}, \qquad v|_{\partial\Omega} = 0.$$

Writing the **Maxwell equations** using the **electric and magnetic** fields, one obtains

$$\begin{bmatrix} \varepsilon & 0 \\ 0 & \mu \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{E}} \\ \dot{\boldsymbol{H}} \end{bmatrix} = \begin{bmatrix} 0 & \nabla\times \\ -\nabla\times & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix}, \qquad \boldsymbol{E}|_{\partial\Omega} = 0.$$

[1] Rashad and Stramigioli, "The port-Hamiltonian structure of continuum mechanics".

Outline

A matter of representation: equivalent formulations for wave equations

Discrete equivalence of Lagrangian and Hamiltonian forms

Equivalence of Lagrangian and port-Hamiltonian discrete systems

Finite element semi-discretization

Classical discretization of the wave equation: find $q_h \in V_{h,0}(\text{grad})$ such that

$$(\psi_h,\, \rho \ddot{q}_h)_\Omega = -(\nabla \psi_h,\, k \nabla q_h)_\Omega \qquad \text{for all } \psi_h \in V_h(\text{grad}).$$

The **discrete Lagrangian** form reads

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{K}\mathbf{q} = 0.$$

The **discrete Hamiltonian** equations are given by

$$\begin{pmatrix} \dot{\mathbf{p}} \\ \dot{\mathbf{q}} \end{pmatrix} = \begin{bmatrix} 0 & -\mathbf{I} \\ \mathbf{I} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{M}^{-1} & 0 \\ 0 & \mathbf{K} \end{bmatrix} \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}, \qquad H = \frac{1}{2}\mathbf{p}^\top \mathbf{M}^{-1}\mathbf{p} + \frac{1}{2}\mathbf{q}^\top \mathbf{K}\mathbf{q}.$$

Remark: we can equivalently rewrite using the velocity

$$\begin{bmatrix} \mathbf{M} & 0 \\ 0 & \mathbf{I} \end{bmatrix} \begin{pmatrix} \dot{\mathbf{v}} \\ \dot{\mathbf{q}} \end{pmatrix} = \begin{bmatrix} 0 & -\mathbf{I} \\ \mathbf{I} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{K} \end{bmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{q} \end{pmatrix}, \qquad H = \frac{1}{2}\mathbf{v}^\top \mathbf{M}\mathbf{v} + \frac{1}{2}\mathbf{q}^\top \mathbf{K}\mathbf{q}.$$

Time integration in Lagrangian dynamics

The finite element discretization of the wave equation leads to the system

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{K}\mathbf{q} = 0.$$

For Lagrangian dynamics the most well known integrator is the Newmark scheme[2]:

$$\begin{aligned}
\mathbf{M}\mathbf{a}^{n+1} + \mathbf{K}\mathbf{q}^{n+1} &= 0, \\
\frac{\mathbf{v}^{n+1} - \mathbf{v}^{n}}{\Delta t} &= \gamma \mathbf{a}^{n+1} + (1-\gamma)\mathbf{a}^{n}, \\
\frac{\mathbf{q}^{n+1} - \mathbf{q}^{n}}{\Delta t} &= \mathbf{v}^{n} + \frac{\Delta t}{2}(2\beta \mathbf{a}^{n+1} + (1-2\beta)\mathbf{a}^{n}).
\end{aligned}$$

Two common choices:

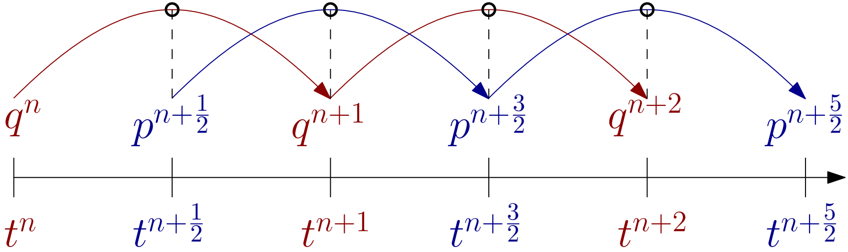
- $\gamma = \frac{1}{2}$, $\beta = 0$: Explicit Newmark (or Leapfrog scheme, or centered differences).
- $\gamma = \frac{1}{2}$, $\beta = \frac{1}{4}$: Implicit Newmark (or implicit midpoint).

[2] Kane et al., "Variational integrators and the Newmark algorithm for conservative and dissipative mechanical systems".

Time integration in Hamiltonian dynamics: Störmer Verlet

The **explicit Newmark** scheme is **equivalent** the **Störmer-Verlet** in Hamiltonian dynamics

$$\frac{\mathbf{p}^{n+\frac{1}{2}} - \mathbf{p}^{n-\frac{1}{2}}}{\Delta t} = -\mathbf{K}\mathbf{q}^n,$$
$$\mathbf{M}\frac{\mathbf{q}^{n+1} - \mathbf{q}^n}{\Delta t} = \mathbf{p}^{n+\frac{1}{2}}.$$

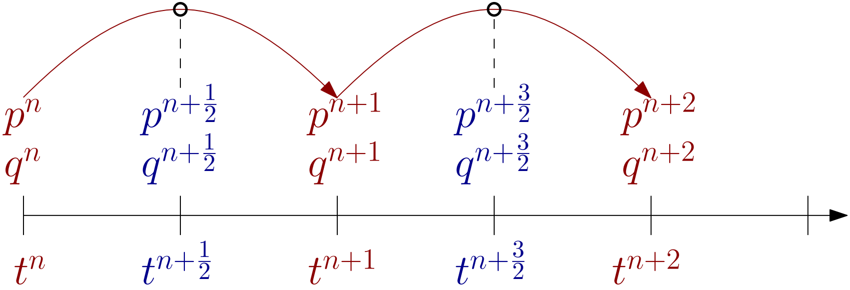


Time integration in Hamiltonian dynamics: implicit midpoint

The **implicit Newmark** scheme scheme is **equivalent** to the **implicit midpoint**

$$\frac{1}{\Delta t}\begin{bmatrix}\mathbf{I} & 0\\ 0 & \mathbf{M}\end{bmatrix}\begin{pmatrix}\mathbf{p}^{n+1}-\mathbf{p}^{n}\\ \mathbf{q}^{n+1}-\mathbf{q}^{n}\end{pmatrix}=\begin{pmatrix}\mathbf{p}^{n+\frac{1}{2}}\\ -\mathbf{K}\mathbf{q}^{n+\frac{1}{2}}\end{pmatrix},$$

where $\mathbf{p}^{n+\frac{1}{2}}=\frac{\mathbf{p}^{n+1}+\mathbf{p}^{n}}{2}$, $\mathbf{q}^{n+\frac{1}{2}}=\frac{\mathbf{q}^{n+1}+\mathbf{q}^{n}}{2}$.



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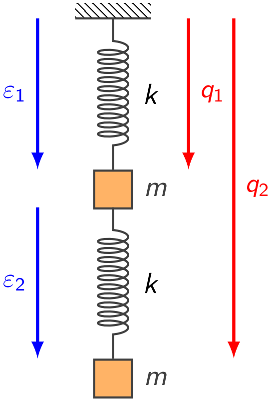
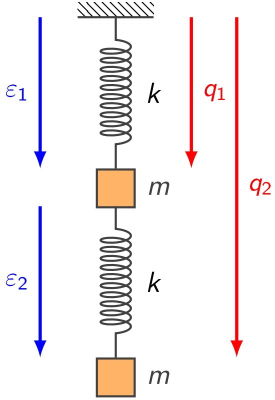
Hamiltonian and port-Hamiltonian formulation of a two dof oscillator[3]



A **two dofs oscillator** is **equivalent** to discretizing the longitudinal wave problem with **two Lagrange finite elements** of degree one and **lumped mass matrix**.

[3] A. J. v. d. Schaft and Maschke, "Port-Hamiltonian Systems on Graphs".

Hamiltonian and port-Hamiltonian formulation of a two dof oscillator[3]



Canonical Hamiltonian formulation

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mathbf{p}\\ \mathbf{q}\end{pmatrix} = \begin{bmatrix}0 & -\mathbf{I}\\ \mathbf{I} & 0\end{bmatrix}\begin{pmatrix}\partial_{\mathbf{p}} H\\ \partial_{\mathbf{q}} H\end{pmatrix}.$$

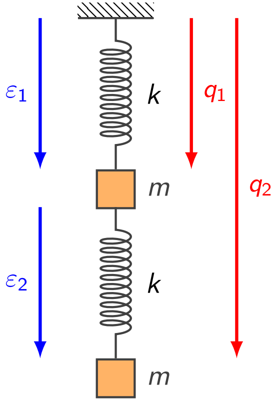
- $\mathbf{p} = \begin{pmatrix}p_1 & p_2\end{pmatrix}^\top = \begin{pmatrix}m\dot{q}_1 & m\dot{q}_2\end{pmatrix}^\top$ linear momenta;
- $\mathbf{q} = \begin{pmatrix}q_1 & q_2\end{pmatrix}^\top$ position of the masses;
- $H = \frac{1}{2}k||\mathbf{D}\mathbf{q}||^2 + \frac{1}{2m}||\mathbf{p}||^2$, where $\mathbf{D} = \begin{bmatrix}1 & 0\\ -1 & 1\end{bmatrix}$.

Remark: notice that

$$U := \frac{1}{2}k||\mathbf{D}\mathbf{q}||^2 = \frac{1}{2}\mathbf{q}^\top\mathbf{K}\mathbf{q}, \qquad \mathbf{K} = k\begin{bmatrix}2 & -1\\ -1 & 1\end{bmatrix}.$$

[3] A. J. v. d. Schaft and Maschke, "Port-Hamiltonian Systems on Graphs".

Hamiltonian and port-Hamiltonian formulation of a two dof oscillator[3]



Interconnection based formulation

A **graph** is associated to the system:

- each node corresponds with an inertial elment;
- each edge corresponds to a spring;

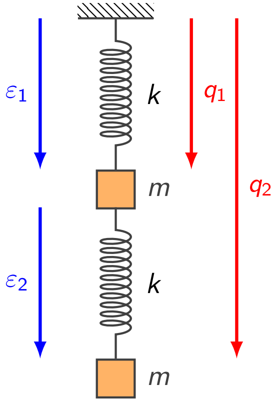
$\mathbf{D}$ is the coincidence matrix and describes the graph topology

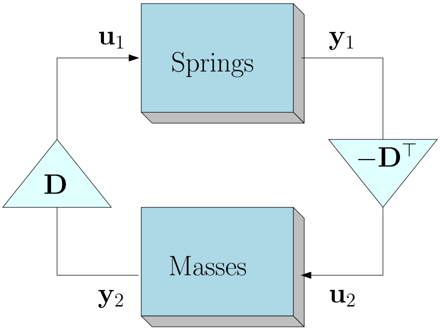
$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\mathbf{p}\\ \boldsymbol{\varepsilon}\end{pmatrix} = \begin{bmatrix}0 & -\mathbf{D}^\top \\ \mathbf{D} & 0\end{bmatrix}\begin{pmatrix}\partial_{\mathbf{p}} H \\ \partial_{\boldsymbol{\varepsilon}} H\end{pmatrix}.$$

- $\boldsymbol{\varepsilon} = (\varepsilon_1 \quad \varepsilon_2)^\top$ spring elongations;
- $H = \frac{1}{2}k||\boldsymbol{\varepsilon}||^2 + \frac{1}{2m}||\mathbf{p}||^2$.

[3] A. J. v. d. Schaft and Maschke, “Port-Hamiltonian Systems on Graphs”.

Hamiltonian and port-Hamiltonian formulation of a two dof oscillator[3]





This formulation corresponds to a mixed finite element discretization.

[3] A. J. v. d. Schaft and Maschke, "Port-Hamiltonian Systems on Graphs".

The primal dual structure

Primal mixed formulation

Find $(v_h, \boldsymbol{\sigma}_h) \in V_h(\mathrm{grad}) \times \boldsymbol{W}_h \subset H(\mathrm{grad}) \times L^2$ such that

$$\begin{aligned} (\psi_h,\, \rho \dot{v}_h)_\Omega &= -(\nabla \psi_h,\, \boldsymbol{\sigma}_h)_\Omega, && \text{for all } \psi_h \in V_h(\mathrm{grad}), \\ (\boldsymbol{\xi}_h,\, c\dot{\boldsymbol{\sigma}})_\Omega &= (\boldsymbol{\xi}_h,\, \nabla v_h)_\Omega, && \text{for all } \boldsymbol{\xi}_h \in \boldsymbol{W}_h. \end{aligned}$$

The primal dual structure

Dual mixed formulation

Find $(v_h, \boldsymbol{\sigma}_h) \in W_h \times \boldsymbol{V}_{h,0}(\mathrm{div}) \subset L^2 \times H_0(\mathrm{div})$ such that

$$\begin{aligned} (\psi_h,\, \rho\dot{v}_h)_\Omega &= (\psi_h,\, \nabla\cdot\boldsymbol{\sigma}_h)_\Omega, && \text{for all } \psi_h \in W_h, \\ (\boldsymbol{\xi}_h,\, c\dot{\boldsymbol{\sigma}})_\Omega &= -(\nabla\cdot\boldsymbol{\xi}_h,\, v_h)_\Omega, && \text{for all } \boldsymbol{\xi}_h \in \boldsymbol{V}_{h,0}(\mathrm{div}). \end{aligned}$$

The primal dual structure

Primal mixed formulation

Find $(v_h, \boldsymbol{\sigma}_h) \in V_h(\mathrm{grad}) \times \boldsymbol{W}_h \subset H(\mathrm{grad}) \times L^2$ such that

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Equivalence of the Lagrangian and port-Hamiltonian formulations

Proposition

Assume that

- the physical coefficients are constant;
- the finite element spaces satisfy the compatibility conditions $\boldsymbol{W}_h \subset \nabla V_h(\text{grad})$,

then the **Lagrangian and port-Hamiltonian primal semi-discretizations are equivalent**.

Proof

Since $\boldsymbol{W}_h \subset \nabla V_h(\text{grad})$ the second equation of the primal formulation holds pointwise

$$c\dot{\boldsymbol{\sigma}}_h = \nabla v_h$$

Integrating in time this equation gives back the classical finite element discretization.

Finite element basis in 1D

For the 1D case, the primal weak formulation is: Find $v \in H^1(\Omega)$, $\sigma \in L^2(\Omega)$

$$
\begin{aligned}
(\xi_v,\, \rho\,\partial_t v)_\Omega &= -(\partial_x \xi_v,\, \sigma)_\Omega, \qquad && \forall\, \xi_v \in H^1(\Omega), \\
(\xi_\sigma,\, c\,\partial_t \sigma)_\Omega &= +(\xi_\sigma,\, \partial_x v)_\Omega, \qquad && \forall\, \xi_\sigma \in L^2(\Omega).
\end{aligned}
$$

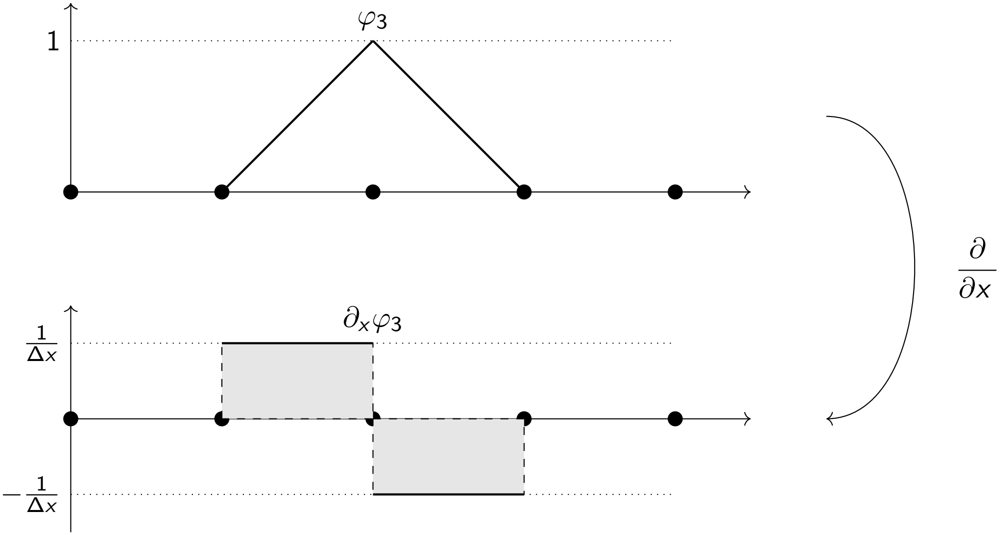
Finite element approximation

$$
\begin{aligned}
v_h(x,t) &= \sum_{i=1}^{N_v} \varphi_v^i(x) v_i(t), \qquad && v_h \in \mathcal{V} = \mathrm{span}\{\varphi_v^1, \ldots, \varphi_v^{N_v}\} \\
\sigma_h(x,t) &= \sum_{i=1}^{N_\sigma} \varphi_\sigma^i(x) \sigma_i(t), \qquad && \sigma_h \in \mathcal{S} = \mathrm{span}\{\varphi_\sigma^1, \ldots, \varphi_\sigma^{N_\sigma}\}.
\end{aligned}
$$

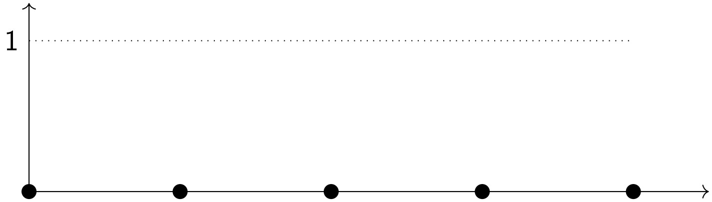
In this formulation

- $v_h \in \mathcal{V} \subset H^1(\Omega)$. **Lagrange elements** can be used.
- $\sigma \in \mathcal{S} \subset L^2(\Omega)$. Which finite element space to choose?

The derivative of a Lagrange space



The Discontinous Galerkin space $\mathbb{DG}_0$



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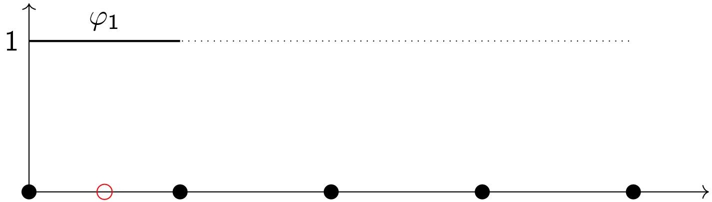

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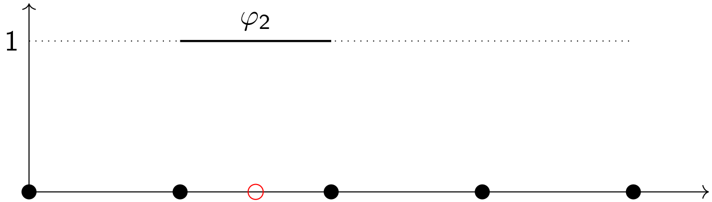

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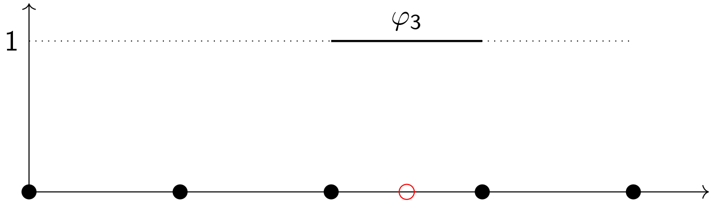

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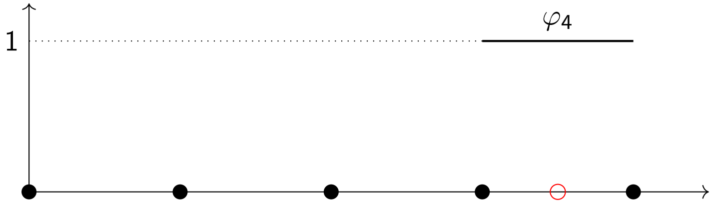

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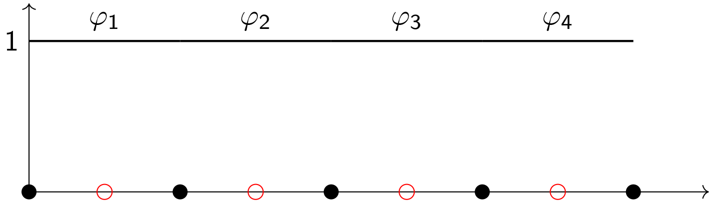


It holds $\partial_x \mathbb{L}_1 \subset \mathbb{DG}_0$. This choice guarantees stability of the formulation.

This is a particular instance of a much more general mathematical construction (subcomplex of an Hilbert complex).

Algebraic equivalence (lowest order FE basis $\mathbb{L}_1$, $\mathbb{DG}_0$)

Largangian form

$$\mathbf{M}\ddot{\mathbf{q}} + \mathbf{K}\mathbf{q} = 0.$$

Primal port-Hamiltonian form

$$\begin{bmatrix} \mathbf{M} & 0 \\ 0 & ch\mathbf{I} \end{bmatrix} \frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} \mathbf{v} \\ \mathbf{s} \end{pmatrix} = \begin{bmatrix} 0 & -\mathbf{D}^\top \\ \mathbf{D} & 0 \end{bmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{s} \end{pmatrix},$$

where h is the mesh-size. $\mathbf{D}$ is the coincidence matrix of the mesh:

$$\mathbf{D} = \begin{bmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix}, \qquad \text{where} \ \ \#\text{elements} = 3$$

Is is related to the stiffness matrix by

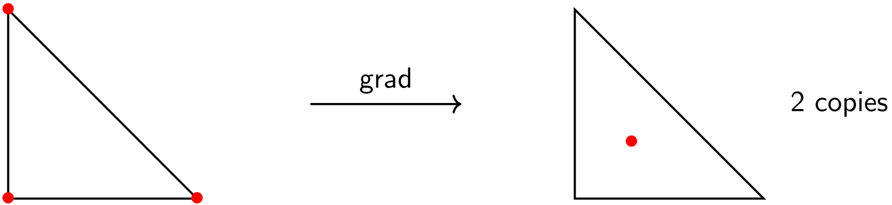
$$\mathbf{K} = \frac{1}{ch}\mathbf{D}^\top\mathbf{D}.$$

Choice of the finite element basis in 2D

Primal formulation: $(\boldsymbol{\xi}_\sigma,\, c\,\partial_t \boldsymbol{\sigma})_\Omega = (\boldsymbol{\xi}_\sigma,\, \mathrm{grad}\, v)_\Omega, \qquad \mathrm{grad}\,\mathcal{V} \subset \mathcal{S}.$

Choice of the finite element basis in 2D

Primal formulation: $(\boldsymbol{\xi}_\sigma,\, c\,\partial_t\boldsymbol{\sigma})_\Omega = (\boldsymbol{\xi}_\sigma,\, \operatorname{grad} v)_\Omega,\qquad \operatorname{grad}\mathcal{V}\subset\mathcal{S}.$



$\mathbb{L}_1$-element:

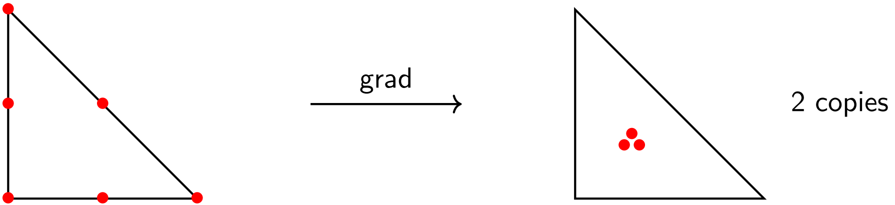
- K = triangle,
- $P_K := \{a_0 + a_1x + a_2y\}$,
- $\Sigma_K := \{$evaluation on vertices$\}$.

$\mathbb{DG}_0$-element:

- K = triangle,
- $P_K := \{a_0\}$,
- $\Sigma_K := \{$evaluation on centroid$\}$.

Choice of the finite element basis in 2D

Primal formulation: $(\boldsymbol{\xi}_\sigma,\, c\,\partial_t \boldsymbol{\sigma})_\Omega = (\boldsymbol{\xi}_\sigma,\, \operatorname{grad} v)_\Omega, \qquad \operatorname{grad} \mathcal{V} \subset \mathcal{S}.$



$\mathbb{L}_2$-element:

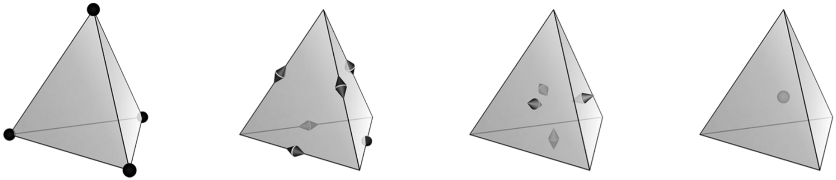
- K = triangle,
- $P_K := \{\cdots + a_3 x^2 + a_4 xy + a_5 y^2\}$,
- $\Sigma_K :=$ {evaluation on vertices and midpoints}.

$\mathbb{DG}_1$-element:

- K = triangle,
- $P_K := \{a_0 + a_1 x + a_2 y\}$,
- $\Sigma_K :=$ {evaluation on 3 nodes}.

Finite element exterior calculus

To obtain stable formulations, finite element exterior calculus can be used.



The Whitney forms (1957).

This framework is well suited port-Hamiltonian systems[4]:

- connection with differential geometry;
- clear separation of topological and metrical operations.

[4] Brugnoli, Rashad, and Stramigioli, "Dual field structure-preserving discretization of port-Hamiltonian systems using finite element exterior calculus".

Time integration and equivalence between different formulations

Proposition

Assume two equivalent time integration method are used for the Lagrangian and port-Hamiltonian form.
The **primal port-Hamiltonian** formulation is **equivalent to the Lagrangian** formulation if the **displacement** is reconstructed via the **trapezoidal rule**

$$\mathbf{q}^{n+1} = \mathbf{q}^{n} + \Delta t \mathbf{v}^{n+\frac{1}{2}}.$$

Conclusion

Classical Lagrangian FE discretization are equivalent to pH discretization when:

- the same time integrator is used;
- the primal FE formulation is used to discretize the port-Hamiltonian dynamics;
- the reduced variable (the displacement) is reconstructed to the trapezoidal rule.

What about the **equivalence when iterative solver are used**[5]?

Recent developments[6] present a unifying framework by introducing Lagrangian subspaces (or Lagrangian submanifolds).

Github repository: https://github.com/a-brugnoli/tutorial-port-hamiltonian

[5] Güdücü et al., "On Non-Hermitian Positive (Semi)Definite Linear Algebraic Systems Arising from Dissipative Hamiltonian DAEs".

[6] Mehrmann and A. v. d. Schaft, "Differential-algebraic systems with dissipative Hamiltonian structure".

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