

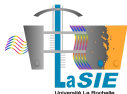
Systemes Hamiltoniens à ports apprentissage et un peu de Dirac



PHS

Vladimir Salnikov

CNRS & La Rochelle University

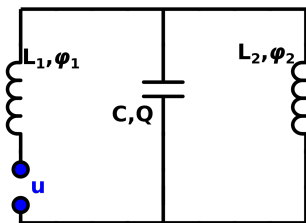


Journée GdR GDM,
IRCAM, 7 mai 2024

In the previous
episodes

Port-Hamiltonian systems.

Example: Electric circuit (L_1, L_2, C) with a controlled port u



$$\begin{cases} \dot{Q} = \varphi_1/L_1 - \varphi_2/L_2 \\ \dot{\varphi}_1 = -Q/C + u \\ \dot{\varphi}_2 = Q/C. \end{cases}$$

$$H = \frac{\varphi_1^2}{2L_1} + \frac{\varphi_2^2}{2L_2} + \frac{Q^2}{2C}$$

Port: input u , output $e = \varphi_1/L_1$.

Port-Hamiltonian system: $\dot{\mathbf{x}} = J(\mathbf{x}) \frac{\partial H}{\partial \mathbf{x}} + g(\mathbf{x})f$ with

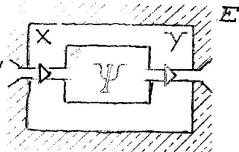
$$\mathbf{x} = \begin{pmatrix} Q \\ \varphi_1 \\ \varphi_2 \end{pmatrix} \quad J = \begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad g = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \begin{matrix} f = u \\ e = \varphi_1/L_1 \end{matrix}$$

$$f_s := -\dot{\mathbf{x}}, \quad e_s := \begin{pmatrix} p_Q \\ p_{\varphi_1} \\ p_{\varphi_2} \end{pmatrix} \equiv \begin{pmatrix} Q/C \\ \varphi_1/L_1 \\ \varphi_2/L_2 \end{pmatrix} \cdot \begin{matrix} \dot{H} \equiv -e_s^T f_s = u\varphi_1/L_1 \Leftrightarrow \\ e_s^T f_s + ef = 0 \\ \Rightarrow \text{almost Dirac} \end{matrix}$$



SYSTEMS ENGINEERING SEMINAR

"PORTS,
ENERGY,
SYSTEMS"



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Professor Henry M. Paynter will present a seminar on the subject, "Ports, Energy and Thermodynamic Systems" on Friday, April 24 at 3:15 p.m. in Room B 103 of the Mechanical Engineering Building.

Dr. Paynter is Assistant Professor of Mechanical Engineering at M.I.T. and Director of the American Center for Analog Computing (a facility of Pi-Square Engineering Company). He is prominently recognized for his work in controls, dynamic systems, analog simulation and related fields. He is the author of very many authoritative papers covering a wide range of topics. He has also done extensive consulting work in industry and government.

Dr. Paynter is a very interesting and stimulating speaker. His viewpoints are novel and thought-provoking.

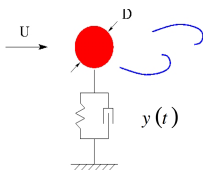
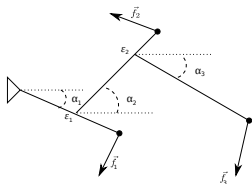
- Henry M. Paynter, Analysis and Design of Engineering Systems, MIT Press, Cambridge, Massachusetts, 1961.

- Jean U. Thoma, Introduction to Bond Graphs and Their Applications, Pergamon Press, Oxford, 1975.

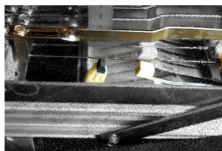
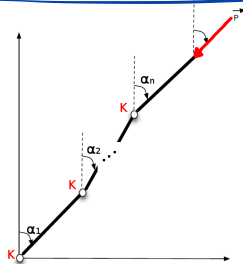
port-Hamiltonian.

Traditional references:

A. van der Schaft, B. Maschke (PHS)



A. Falaize
Py PHS



Proof?

Conjecture (VS): Everything is port-Hamiltonian.

Geometry: (almost) Dirac structures



Philosophy



https://math.ucr.edu/home/baez/week292.html

	displacement q	flow q'	momentum p	effort p'
Mechanics (translation)	position	velocity	momentum	force
Mechanics (rotation)	angle	angular velocity	angular momentum	torque
Electronics	charge	current	flux linkage	voltage
Hydraulics	volume	flow	pressure momentum	pressure
Thermodynamics	entropy	entropy flow	temperature momentum	temperature
Chemistry	moles	molar flow	chemical momentum	chemical potential

J.-M. Souriau's thermodynamics,
or better: C.-M. Marle <https://arxiv.org/abs/1608.00103>

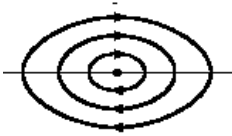

Episode 1: Almost Dirac structures for PHS

Very classical story

Verlet '67
Yoshida '80s

Cohomology



<p>Canonical case: given $H: T^*Q \rightarrow \mathbb{R}$</p> $\dot{\mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{q}}$	<p>Symplectic geometry</p> $\omega = \sum_i dp_i \wedge dq^i$ $\iota_{X_H} \omega = dH$	
<p>More general case: given $H: M \rightarrow \mathbb{R}$ and an antisymmetric $J(\mathbf{x})$</p> $\dot{\mathbf{x}} = J(\mathbf{x}) \frac{\partial H}{\partial \mathbf{x}}$	<p>Poisson geometry $\{\cdot, \cdot\}$ on $C^\infty(M)$</p> $X_H = \{H, \cdot\}$ $\dot{\mathbf{x}} = \{H, \mathbf{x}\}$	

Oscar Cosserat, 2022

No variational formulation

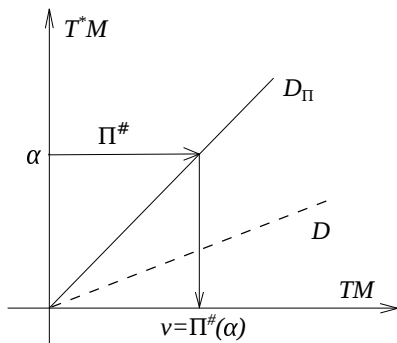
Geometry behind: Courant algebroids, Dirac structures

On $\mathbb{T}M = TM \oplus T^*M$ (or more generally $E \oplus E^*$)

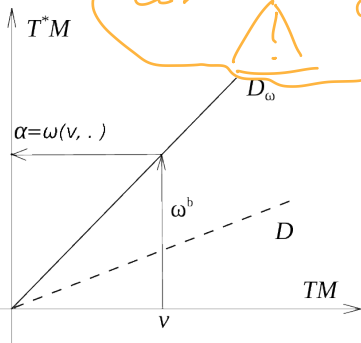
Symmetric pairing: $\langle v \oplus \eta, v' \oplus \eta' \rangle = \eta(v') + \eta'(v)$,

Dorfman bracket: $[v \oplus \eta, v' \oplus \eta']_D = [v, v']_{\text{Lie}} \oplus (\mathcal{L}_v \eta' - d\eta(v'))$.

A *Dirac structure* \mathcal{D} is a maximally isotropic (Lagrangian) subbundle of $\mathbb{T}M$ closed w.r.t. $[\cdot, \cdot]_D$



$$\mathcal{D}_\Pi = \text{graph}(\Pi^\#) = \{(\Pi^\# \alpha, \alpha)\}$$



$$\mathcal{D}_\omega = \text{graph}(\omega^b) = \{(v, \iota_v \omega)\}$$

Dirac paths

(Cossierat, Laurend-Geuzans, Kobou,
Ryckin, VS)

Theorem 1. Let $D \subset \mathbb{T}M$ be a Dirac structure over M ,
 $H \in C^\infty(M)$ be a Hamiltonian function and γ a path on M .



Assume that the basic 2-class $[\omega_D]$ vanishes, and let $\theta \in \Gamma(D^*)^{\text{hor}}$ be such that $d_D\theta = \omega_D$, then the following statements are equivalent:

- (i) The path γ is a Hamiltonian curve, i.e. $(\dot{\gamma}(t), dH_{\gamma(t)}) \in D$ for all t .
- (ii) All Dirac paths $\zeta : I \rightarrow D$ over γ (i.e. $\rho(\zeta) = \dot{\gamma}$) are critical points among the Dirac paths with the same end points of the following functional:

$$\zeta \mapsto \int_I (\theta_{\gamma(t)}(\zeta(t)) + H(\gamma(t))) dt \quad (1)$$

Implicit Lagrangian systems with magnetic terms

Theorem 2. Let $D \subset \mathbb{T}Q$ be a Dirac structure and $L : TQ \rightarrow \mathbb{R}$ a Lagrangian. Assume that the 2-form $\omega_D \in \Gamma(\Lambda^2 D^*)^{hor}$ admits a basic primitive $\theta \in \Gamma(D^*)^{hor}$. Then for $q : I \rightarrow Q$ the following are equivalent:

- a) There exists a Dirac path $\zeta : I \rightarrow D$ such that $\rho(\zeta) = \dot{q}$ which is the critical point among Dirac paths with the same end points of

$$\int_I (L(\rho(\zeta(t))) + \theta(\zeta(t))) dt. \quad (2)$$

- b) For all $t \in I$, the following condition holds.

$$\left(\frac{\partial}{\partial t} \mathbb{F}L(\dot{q}(t)), \mathcal{D}_{\dot{q}(t)} L \right) \in \mathbb{D} = e^{\Omega} \pi^! D. \quad (3)$$

Task: Dirac integrator

Episode 2: Conjecture ?

Port-Hamiltonian systems (PHS): definition and features

General form:

$$\dot{\mathbf{x}} = (J(\mathbf{x}) - R(\mathbf{x})) \frac{\partial H}{\partial \mathbf{x}} + w(\mathbf{x}) \mathbf{u}. \quad (1)$$

- Symplectic Hamiltonian systems are PHS

$$J = J_D = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$$

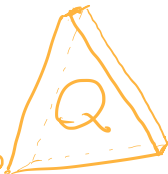
- Poisson Hamiltonian systems are PHS

$$J = J_W = \begin{pmatrix} J_D & 0 \\ 0 & \Phi(\mathbf{y}) \end{pmatrix}$$

- PHS + PHS \Rightarrow PHS

$$\left(\begin{array}{ccc|ccc} J_1 - R_1 & & & x & 0 & x \\ & & & 0 & x & 0 \\ & & & 0 & 0 & 0 \\ \hline x & x & 0 & & & \\ & & & J_2 - R_2 & & \\ 0 & x & 0 & & & \end{array} \right)$$

- PHS \Rightarrow PHS + PHS ?? Not unique!



Conjecture in a reasonable form

$$W(x, q, \dot{q}) = W_2 + W_1 + W_0$$

Dirac's FGB
Algebraisches
Q-System

$q \in \mathbb{R}^N$
 $\mathcal{P} = F(t, q, \dot{q}) \cdot \dot{q}$

g independent for det
 $Q = F$

$$\frac{d}{dt} \left(\frac{\partial W}{\partial \dot{q}} \right) - \frac{\partial W}{\partial q} = Q$$

$$Q = \frac{\partial V}{\partial q} + R$$

$W = W_2$

$$\left[\frac{d}{dt} \left(\frac{\partial W_2}{\partial \dot{q}} \right) - \frac{\partial W_2}{\partial q} \right] \dot{q} = Q \dot{q} \quad \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = R$$

$L = W - V$

$\int_{\Sigma} f(M) \cdot v(M) d\mu$

$W: TM \rightarrow \mathbb{R}$

$$\frac{dp}{dt} = \frac{\partial H}{\partial q} + R \quad \frac{dq}{dt} = -\frac{\partial H}{\partial p}$$

$\frac{\partial W}{\partial \dot{q}} + \frac{\partial W}{\partial q} \dot{q}$
 $\int_{\Sigma} f(M) \frac{\partial W}{\partial \dot{q}} \delta q d\mu$

$\frac{dH}{dt} = \frac{\partial H}{\partial q} \dot{q} + \frac{\partial H}{\partial p} \dot{p}$
 $= \frac{\partial H}{\partial p} R$

$\frac{\partial W}{\partial \dot{q}} \in T^*M$
 $R \in T(T^*M)$

$$\int \underline{\text{str}}(b, F_{Ad})$$

Port-Hamiltonian systems (PHS): definition and features

General form:

$$\dot{\mathbf{x}} = (J(\mathbf{x}) - R(\mathbf{x})) \frac{\partial H}{\partial \mathbf{x}} + w(\mathbf{x}) \mathbf{u}. \quad (1)$$

- Symplectic Hamiltonian systems are PHS

$$J = J_D = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$$

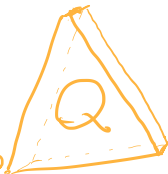
- Poisson Hamiltonian systems are PHS

$$J = J_W = \begin{pmatrix} J_D & 0 \\ 0 & \Phi(\mathbf{y}) \end{pmatrix}$$

- PHS + PHS \Rightarrow PHS

$$\left(\begin{array}{ccc|ccc} J_1 - R_1 & & & x & 0 & x \\ & & & 0 & x & 0 \\ & & & 0 & 0 & 0 \\ \hline x & x & 0 & & & \\ & & & J_2 - R_2 & & \\ 0 & x & 0 & & & \end{array} \right)$$

- PHS \Rightarrow PHS + PHS ?? Not unique!



CA

$$\dot{\mathbf{X}} = \mathbf{F}(\mathbf{X}) \quad (2)$$

Episode 3: Notilus aka intelligent accounting

Reconstructing PHS

Input data: a system of differential equations of form (2).

1. Reconstruct the connectivity graph of the PHS, i.e., identify the nodes and their interconnections.

2. Label the graph, i.e., identify or select the symplectic/Poisson structure and the corresponding Hamiltonian.

3. Label the connections among the nodes, i.e., identify the ports.

Output data: the graph (set of PHS nodes and ports) labeled in notation (1).

Recovering the PHS structure II

II. For each group:

1. Construct (or select from a catalog constructed in advance) all the symplectic and Poisson structures of suitable size.
2. From the internal variables select the maximal combination of terms, preserving one of the structures from the previous step.
3. If the cohomology of the selected structures is non-trivial, check if the selected combination belongs to the trivial class.
4. Construct the Hamiltonian, corresponding to the selected combination of terms. If this step results in unreasonably complicated symbolic computations, come back to steps 1.-2., dropping highly non-linear terms from the selection.

After that, for each group of variables the components of a Hamiltonian flow are spelled-out.

Recovering PHS structure I: matrices

$$\left(\begin{array}{ccc|ccc} J-R_1 & & & * & 0 & * \\ & * & & 0 & * & \\ & & & 0 & 0 & * \\ \hline 0 & 0 & 0 & & & \\ * & * & 0 & J_2-R_2 & & \\ 0 & * & 0 & & & \end{array} \right)$$

Proof of concept OK

tests $n=10$

$m=2, 3, 4$

Everything at
most quadratic

Conclusion: in principal OK

Scalability?

APPENDIX A: SOME TECHNICAL DETAILS

The data considered in Section 3 were processed by a fully convolutional neural network, which had two convolutional layers (activation layer and dropout layer) and a sample normalization layer. The Adam function was chosen as the optimization function, and the root mean square was chosen as the loss function.

The Adam optimizer adjusted the weights according to the following rule:

$$w_t = w_{t-1} - \eta \frac{\hat{m}_t}{\sqrt{\hat{v}_t + \epsilon}}$$

where w_t are the weights of the t th layer and v_t is the step parameter.

$$\hat{m}_t = \frac{m_t}{1 - \beta_1^t}$$

$$\hat{v}_t = \frac{v_t}{1 - \beta_2^t}$$

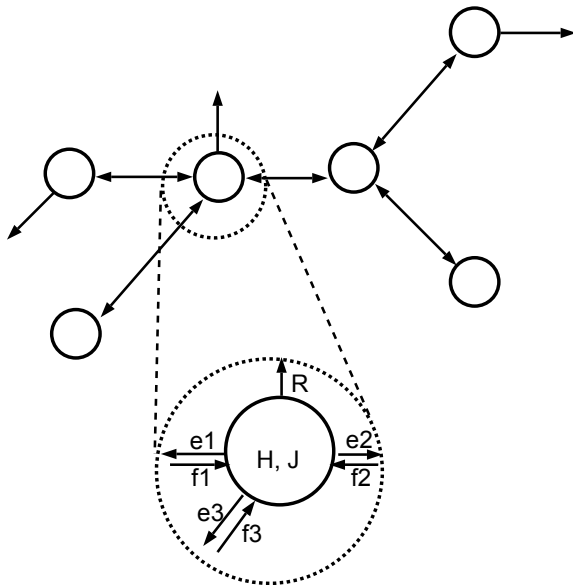
$$m_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t$$

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$$

where g_t is the gradient on the current mini-sample, β_1 are hyperparameters with initial values close to 1, while variables m_t and v_t are the mean and biased deviations for the gradients of the loss functions.

The number of filters for each convolution layer was 6428. The number of "trained" parameters was 175162.

Port-Hamiltonian systems as decorated graphs



Recovering the PHS structure I

Input data: a system of differential equations in the form $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$

- I. From the right hand sides, recover the structure of the graph of the PHS.

After that, the variables x_i are split into groups (vertexes of the graph), and the terms in the right hand sides are separated to internal ones (i.e. depending only on variables of their “proper” group) and external ones (all the others).

↳ Graph pooling
(E.g. Map Equation)

Recovering the PHS structure III

III. Identify the ports:

1. The terms not selected in step II.2. are declared internal ports, associate “virtual” vertices to them.
2. To external terms for each group (responsible for interactions) assign an edge in the resulting graph.

Details:

- V.Salnikov, A.Falaize, D.Loziienko. Learning port-Hamiltonian systems - algorithms, Computational Mathematics and Mathematical Physics, 2023.
- V. Salnikov, Port-Hamiltonian systems: structure recognition and applications, Programming and Computer Software, Volume 50, 2, 2024

Learning the PHS structure – some remarks

- First step – Machine Learning methods.

Proof of concept – OK.

Hamiltonian VS generic training ? *Need hands*  *Success criteria?*

- Second step – “catalog” of symplectic / Poisson structures, computation of cohomologies and compatible vector fields.
- Maybe a new way of defining **canonical forms of systems of differential equations.**



Merci pour votre attention!

