Poisson-Dirac Neural Networks for Modeling Coupled Dynamical Systems across Domains

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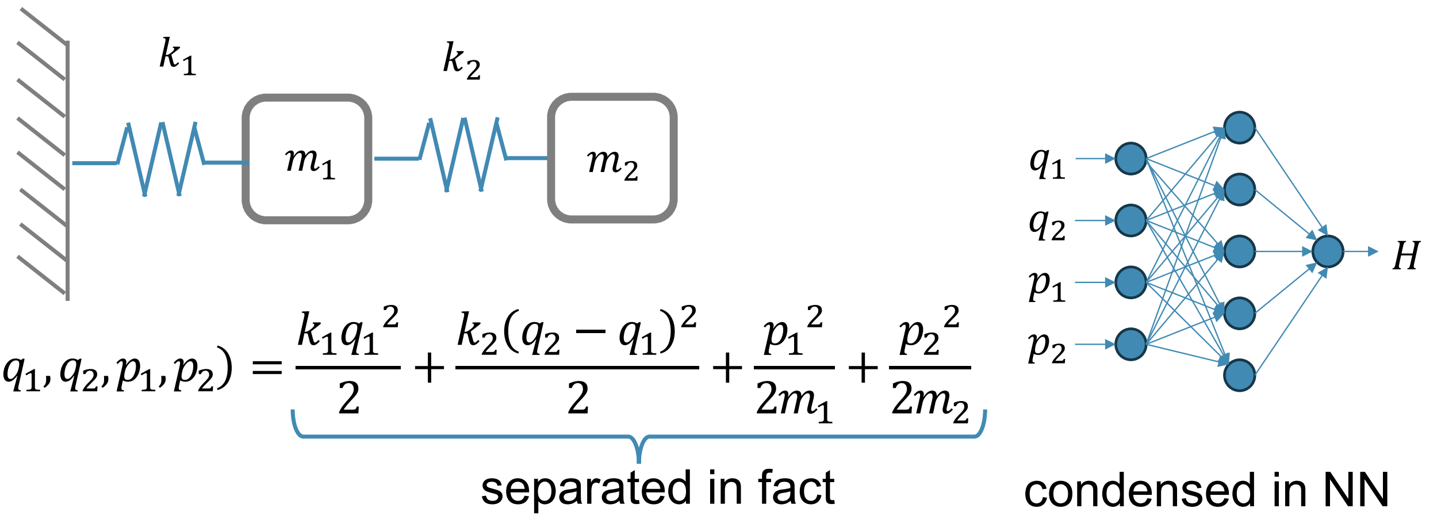
Deep Learning for Dynamical Systems

Deep learning for Data-driven simulators

- **Deep learning can build simulators from observations** by learning the underlying differential equations $\dot{x} = f(x)$.
  - crucial for the design & control of circuit, vehicle & robot.
- **Existing methods:**
  - Neural ODEs for general ODEs [1]
  - HNNs for *conservative systems* [2]
  - Dissipative SymODENs for *controls and dissipations* [3]
  - CHNNs and PNNs for *constraints and degeneracy* [4,5]

Limitations

- **Narrowed scope:** Focuses only on mechanical systems and address only limited aspects as above
- **Monolithic structure:** Treats a system as a single entity, and embeds the interactions between sub-components in a neural network, hindering interpretability



$$H(q_1,q_2,p_1,p_2) = \underbrace{\frac{k_1{q_1}^2}{2} + \frac{k_2(q_2-q_1)^2}{2} + \frac{{p_1}^2}{2m_1} + \frac{{p_2}^2}{2m_2}}_{\text{separated in fact}}$$

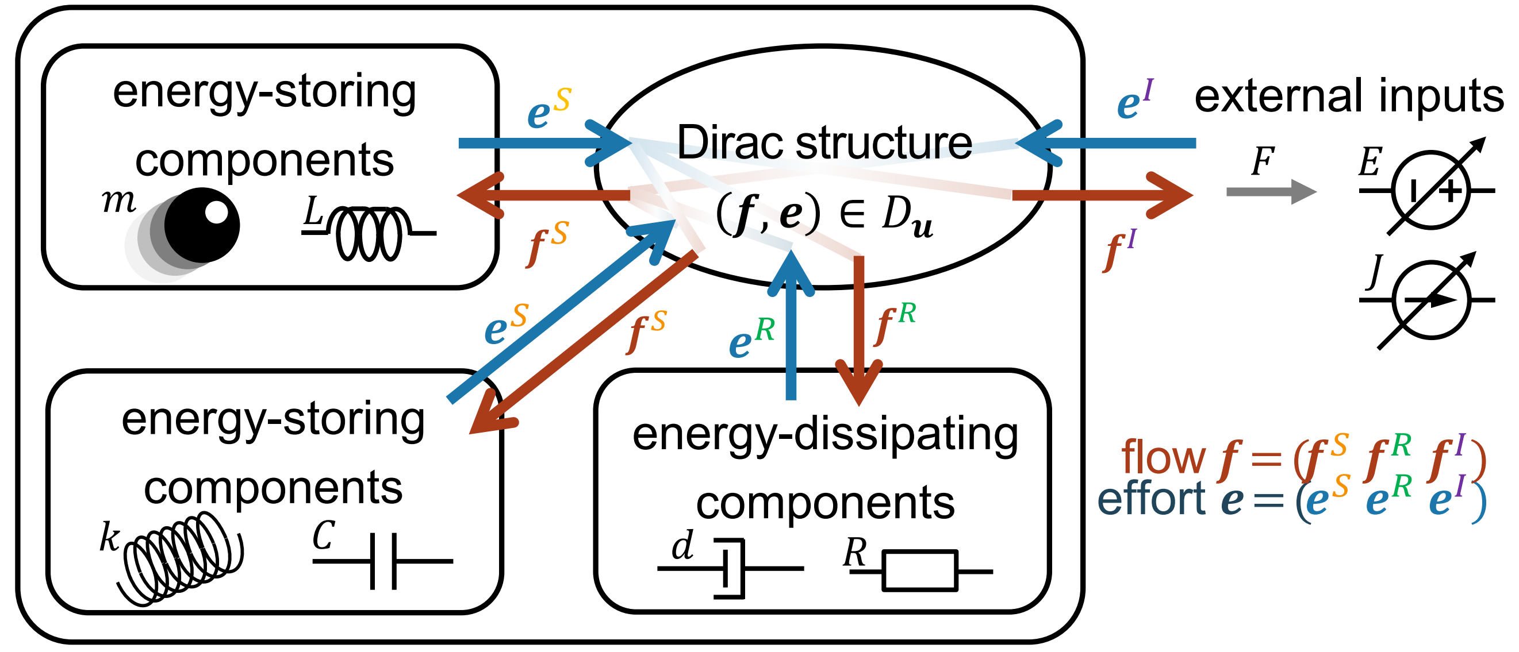
condensed in NN

Key Contributions

- **Unified Modeling:**
  - Handles diverse physics domains (mechanical, electrical, hydraulic, etc.) and their interactions (multiphysics).
  - Handles various aspects, including energy conservation, dissipation, external inputs, and degeneracy.
- **Interpretability:** Explicitly learns and identifies coupling patterns and component-wise characteristics from data.
- **Robustness**: Improves modeling accuracy and long-term prediction stability by separating the interactions from component-wise behavior.

Poisson-Dirac Formulation

Background Theory



flow $f = (f^S\ f^R\ f^I)$
effort $e = (e^S\ e^R\ e^I)$

- **Intuitive explanations**
  - **Flow** f: inputs to components (ex. velocity for a spring)
  - **Effort** e: outputs form components (ex. force for a spring)
  - **Dirac Structure** D: defines the interactions.
- **Dirac Structure** D: unifies symplectic form and Poisson bivector, and defines Hamiltonian systems, Poisson systems, and port-Hamiltonian systems. [6,7]
  - A vector bundle $\mathcal{F} \oplus \mathcal{E}$ over a manifold $\mathcal{M}$
  - Fibers at u: $\mathcal{F}_u = \mathcal{F}_u^S \oplus \mathcal{F}_u^R \oplus \mathcal{F}_u^I, \mathcal{E}_u = \mathcal{E}_u^S \oplus \mathcal{E}_u^R \oplus \mathcal{E}_u^I$
  - Flows $f = (f^S\ f^R\ f^I) \in \mathcal{F}$ and efforts $e = (e^S\ e^R\ e^I) \in \mathcal{E}$
  - A bundle map (defined by a bivector): $B_u^\#: \mathcal{F}_u \to \mathcal{E}_u$
  - Dirac structure $D \subset \mathcal{F} \oplus \mathcal{E},\ D_u = \{(f,e) \in \mathcal{F}_u \times \mathcal{E}_u | f = B^\# e\}$
- **Poisson-Dirac formulation of mechanics**
  - Hamiltonian $H: \mathcal{M} \to \mathbb{R}$, state update: $f^S = \dot{u}$
  - Efforts $e^S = \mathrm{d}H,\ e^R = R_u(f^R),\ e^I(t) = F(t)$
  - $\big((f^S(t), f^R(t), f^I(t)), (e^S(t), e^R(t), e^I(t))\big) \in D_{u(t)}$

$$\Rightarrow \begin{bmatrix} \dot{u} \\ f^R \\ f^I \end{bmatrix} = B_u^\# \begin{bmatrix} \nabla H(u) \\ R_u(f^R) \\ F(t) \end{bmatrix}$$

Target Systems

Domain	Mechanical		Rotational		Electro-Magnetic		Hydraulic
Subdomain	Potential	Kinetic	Potential	Kinetic	Electric	Magnetic	Potential
flow (input)	velocity	force	angular velocity	torque	current	voltage	volume flow rate
effort (output)	force	velocity	torque	angular velocity	voltage	current	pressure
state	displacement	momentum	angle	angular momentum	electric charge	magnetic flux	volume
energy-storing	spring	mass	(potential)	inertia	capacitor	inductor	hydraulic tank
energy-dissipating	damper	-	friction	-	resistor	resistor	-
external input	external force	moving boundary	external torque	-	voltage source	current source	incoming fluid flow

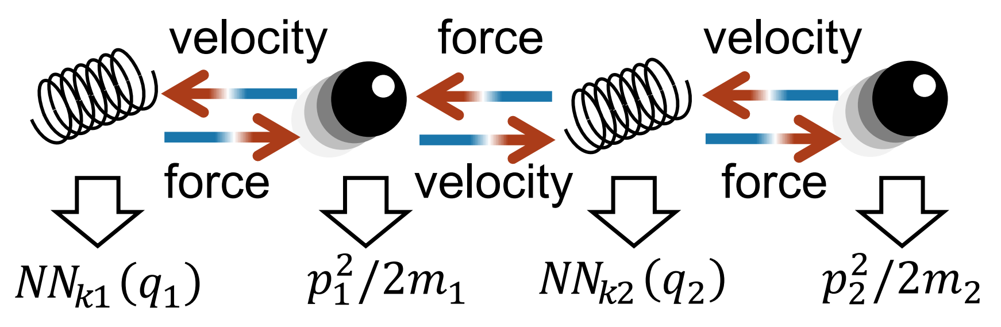
Poisson-Dirac Neural Networks

Implementations

- **Components:**
  - Nonlinear, energy-storing: An NN-based energy function H.
  - Linear, energy-storing: A learnable quadratic function H.
  - Nonlinear, energy-dissipating: An NN-based map R_u.
- **Dirac Structure:**
  - A learnable skew-symmetric matrix $B_u^\#$.
  - Fix elements of $B_u^\#$ for incompatible couplings at zero. (e.g., mass and mass, spring and external force)
- **Example:**

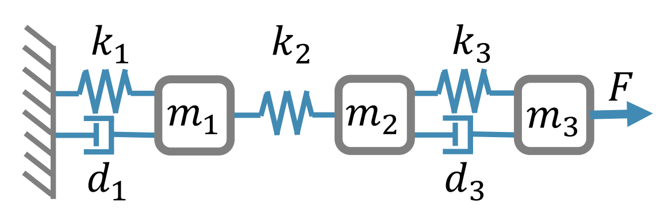
$$B_u^\# = \begin{array}{c} \\ \\ \\ \\ \end{array}\begin{array}{cccc} q_1 & q_2 & p_1 & p_2 \end{array}$$

$$B_u^\# = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

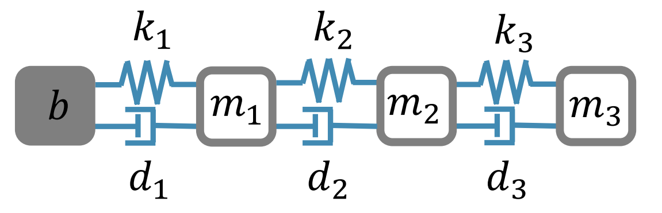


separately modeled

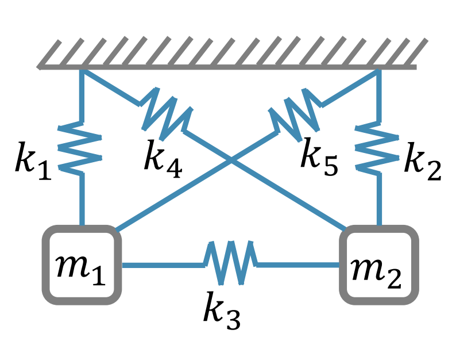
Datasets



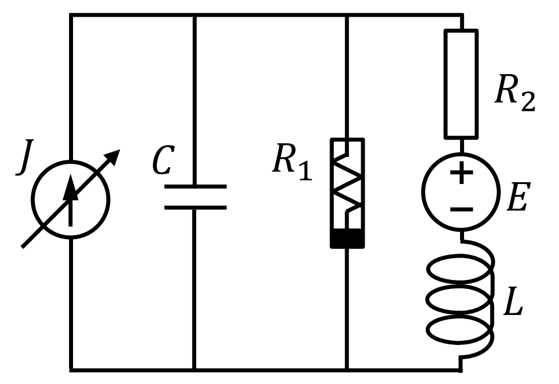
(a) with external force



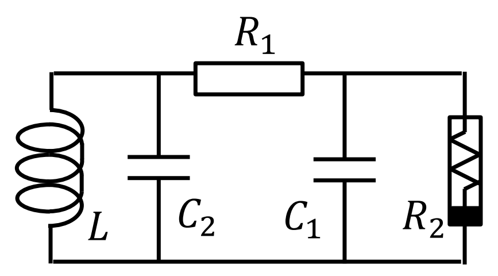
(b) with moving boundary



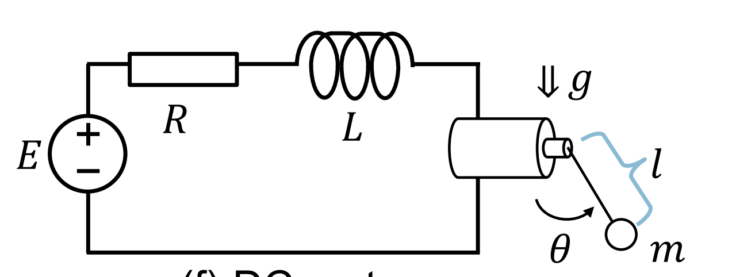
(c) with redundancy



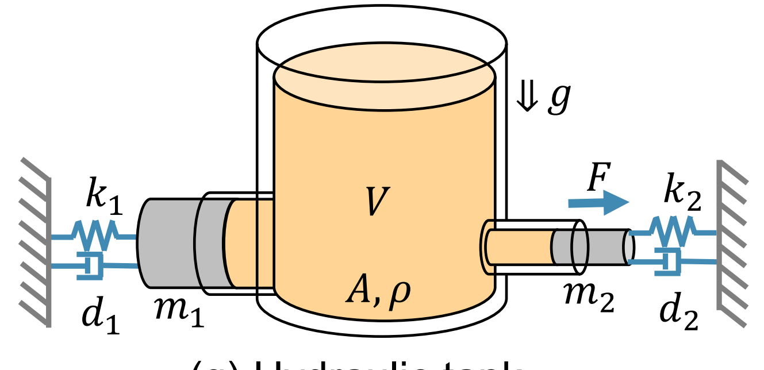
(d) FitzHugh-Nagumo model



(e) Chua's circuit



(f) DC motor



(g) Hydraulic tank

Experiments and Results

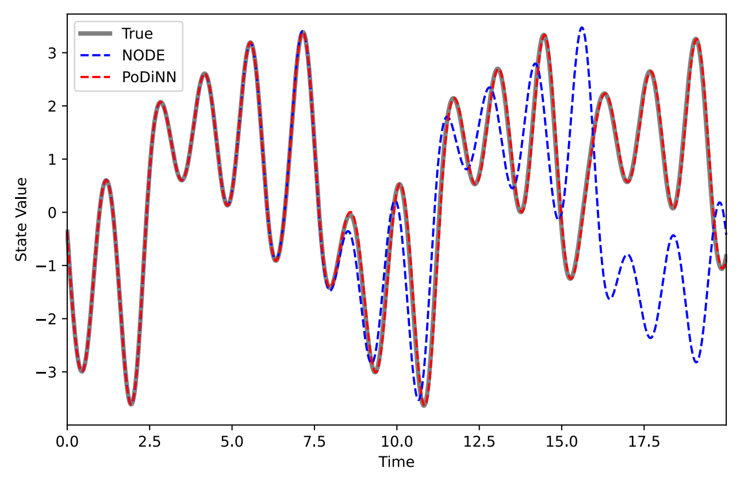
Results

	Mass-Spring-Damper Systems					
Dataset	(a) with external force		(b) with moving boundary		(c) degeneracy	
Subdomain	MSE↓	VPT↑	MSE↓	VPT↑	MSE↓	VPT↑
Neural ODE	7.68 ± 1.07	0.097 ± 0.008	5.02 ± 0.56	0.135 ± 0.052	> 1000	0.099 ± 0.004
HNN Variants*	8.31 ± 0.56	0.104 ± 0.017	5.92 ± 0.12	0.001 ± 0.000	> 100	0.000 ± 0.000
PoDiNN	$\mathbf{4.33} \pm 0.26$	$\mathbf{0.622} \pm 0.002$	$\mathbf{0.26} \pm 1.12$	$\mathbf{0.856} \pm 0.015$	$\mathbf{0.11} \pm 0.02$	$\mathbf{0.863} \pm 0.017$
	$\times 10^{-1}$	$\theta = 10^{-3}$	$\times 10^{-2}$	$\theta = 10^{-4}$	$\times 10^{-1}$	$\theta = 10^{-3}$

	Electric Circuits				Multiphysics			
	(d) FitzHugh-Nagumo		(e) Chua's circuit		(f) DC motor		(g) Hydraulic Tank	
	MSE↓	VPT↑	MSE↓	VPT↑	MSE↓	VPT↑	MSE↓	VPT↑
Neural ODE	48.96 ± 17.43	0.322 ± 0.041	14.74 ± 1.33	0.287 ± 0.016	16.03 ± 5.15	0.276 ± 0.168	30.62 ± 8.22	0.045 ± 0.010
PoDiNN	$\mathbf{1.64} \pm 1.37$	$\mathbf{0.649} \pm 0.072$	$\mathbf{9.21} \pm 0.83$	$\mathbf{0.469} \pm 0.010$	$\mathbf{2.11} \pm 2.90$	$\mathbf{0.923} \pm 0.013$	$\mathbf{5.42} \pm 3.65$	$\mathbf{0.918} \pm 0.013$
	$\times 10^{-4}$	$\theta = 10^{-3}$	$\times 10^{-1}$	$\theta = 10^{-3}$	$\times 10^{-3}$	$\theta = 10^{-4}$	$\times 10^{-2}$	$\theta = 10^{-4}$

Identification

- **(e) Chua's Circuit**
  - **Dynamics**



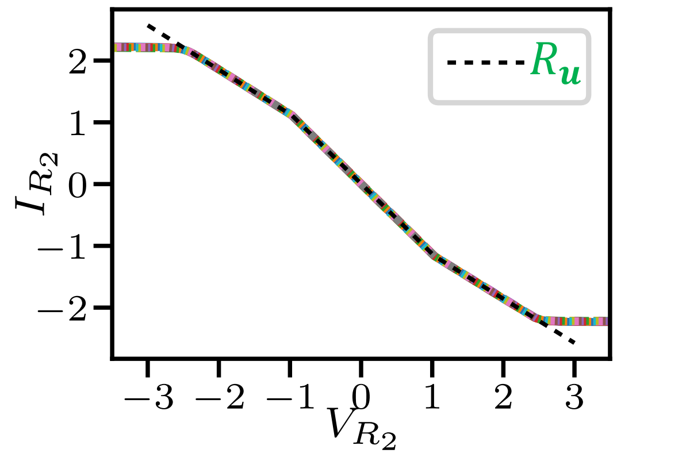
Prediction result of L

- **Coupling patters**

$$\begin{array}{c|ccc} & L & R_1 & R_2 \\ \hline C_1 & 0 & c & -d \\ C_2 & a & -b & 0 \end{array}$$

Identified submatrix of $B_u^\#$
The sign implies the direction.

- **Component-wise characteristics**



Identified characteristic of R_2
Each color represents one trial.

- **(b) Mass-Spring-Damper**
  - **Number of unobservable components**

# of Dampers	Training	Test
$n_d = 0$	0.005 ± 0.000	0.000 ± 0.000
$n_d = 1$	0.009 ± 0.002	0.001 ± 0.000
$n_d = 2$	0.015 ± 0.000	0.001 ± 0.000
$n_d = 3$	$\mathbf{0.925} \pm 0.007$	$\mathbf{0.581} \pm 0.040$
$n_d = 4$	$\mathbf{0.932} \pm 0.010$	$\mathbf{0.597} \pm 0.058$
$n_d = 5$	$\mathbf{0.935} \pm 0.006$	$\mathbf{0.600} \pm 0.035$
	$\theta = 10^{-4}$	$\theta = 10^{-4}$

VPTs with varying # of unobservable dampers
An insufficient number leads to a poor score, even for training datasets.

- **(c) Mass-Spring**
  - **Coupling patterns**

$$\begin{array}{c|cccc} & \overbrace{\quad\quad}^{m_1} & & \overbrace{\quad\quad}^{m_2} & \\ \hline k_1 & 1 & 0 & 0 & 0 \\ & 0 & 1 & 0 & 0 \\ k_2 & 0 & 0 & 1 & 0 \\ & 0 & 0 & 0 & 1 \\ k_3 & -1 & 0 & 1 & 0 \\ & 0 & -1 & 0 & 1 \end{array}$$

Identified submatrix of $B_u^\#$
The sign implies the direction.
Redundancy is found.

- **(g) Hydraulic Tank**
  - **Coupling patterns**

$$\begin{array}{c|cc} & m_1 & m_2 \\ \hline k_1 & 1 & 0 \\ k_2 & 0 & 1 \\ A & 1 & -0.3 \\ d_1 & a & 0 \\ d_2 & 0 & b \\ F & 0 & c \end{array}$$

Identified submatrix of $B_u^\#$
The cylinder sizes are identified as coupling strengths

Reference

[1] Chen et al., NeurIPS, 2018.
[2] Greydanus et al., NeurIPS, 2019.
[3] Zhong et al., ICLRW, 2020.
[4] Finzi el al., ICML, 2020.
[5] Jin et al., TNNLS, 2023.
[6] Schaft & Jeltsema, 2014.
[7] Yoshimura & Marsden, JGP, 2006.