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

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Background

Goal: Predict physical phenomena without governing equations

Ex). Neural ODEs learn the dynamics f of a system $\dot{\boldsymbol{x}} = f(\boldsymbol{x})$ by deep learning, where $\boldsymbol{x}$ is the state of the system .

[1] Chen+, NeurIPS, 2018

- Overly general models neglect underlying principles such as energy conservation.

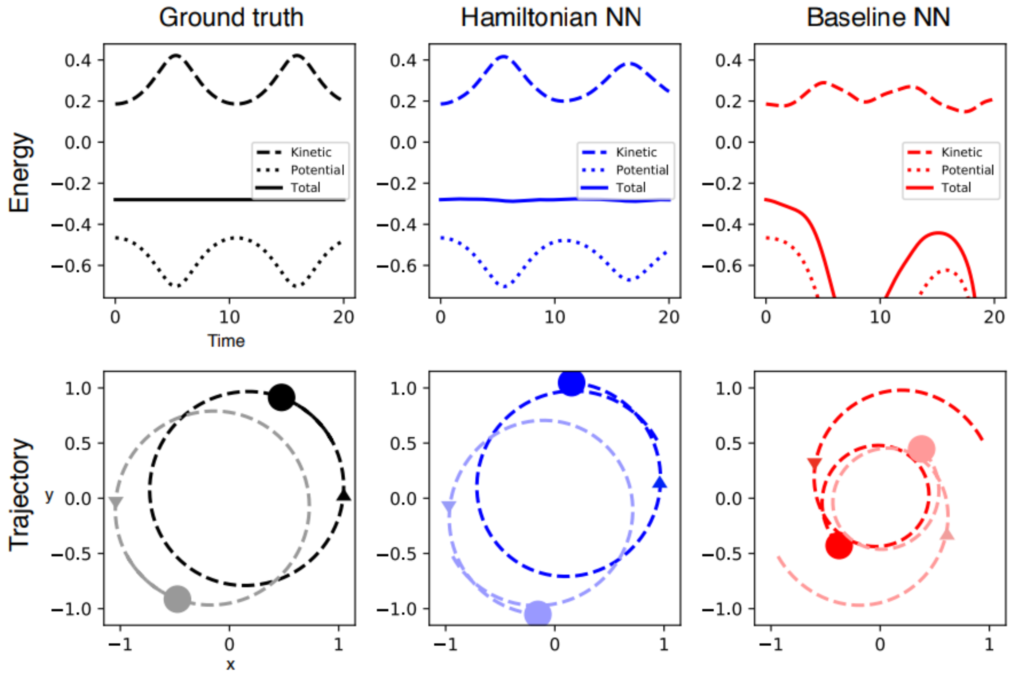
Related Work

Hamiltonian Neural Networks (HNNs)

[2] Greydanus+, NeurIPS, 2019
[3] Zhong+, ICLR Workshop, 2020
[4] Jin+, IEEE TNNLS, 2022

- describe the dynamics by Hamilton's equations, using generalized coordinate $\boldsymbol{q}$ and momenta $\boldsymbol{p}$ as the state.

$$\begin{pmatrix} \dot{\boldsymbol{q}} \\ \dot{\boldsymbol{p}} \end{pmatrix} = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \nabla H(\boldsymbol{q}, \boldsymbol{p})$$



- learn Hamiltonian H by a neural network.

  → improves long-term prediction.

- have several extensions.

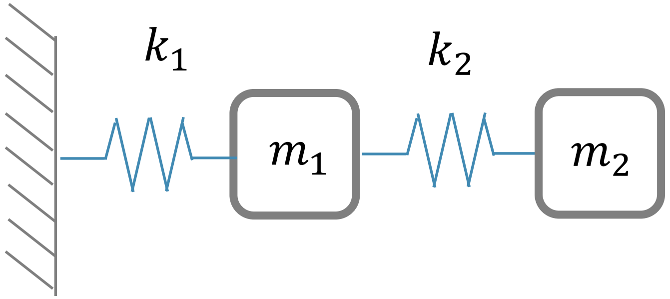
  Ex). Dissipative SymODENs, Poisson Neural Networks (PNNs)

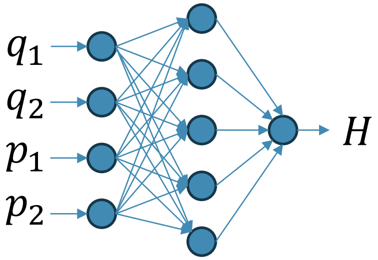
Related Works

Limitation 1

- The interactions of the elements that compose the system are implicitly embedded in neural networks.
  → leading to reduced interpretability and prediction performance.

Ex). Modeling mass-spring system by HNNs.





$$H(q_1, q_2, p_1, p_2) = \frac{k_1 {q_1}^2}{2} + \frac{k_2 (q_2 - q_1)^2}{2} + \frac{{p_1}^2}{2m_1} + \frac{{p_2}^2}{2m_2}$$

→ treating the system as a single, monolithic entity

Related Works

Limitation 2

- The narrowed scope of applications.

Model	Degeneracy	Dissipation	External Input	Multiphysics
HNN	✗	✗	✗	✗
Dis. SymODEN	✗	✓	*	✗
PNN	✓	✗	✗	✗
PoDiNN (proposed)	✓	✓	✓	✓

* Available only for external force on mass.

Proposed Method

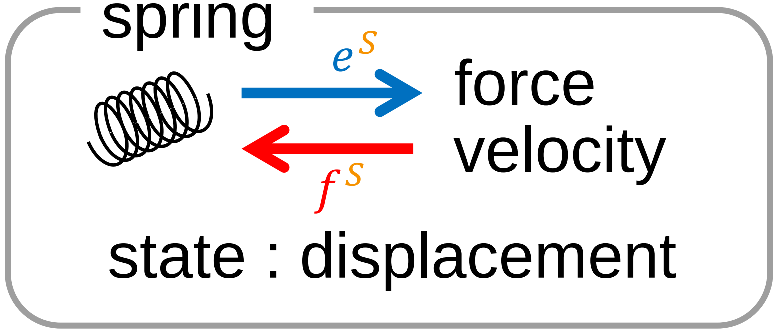
Poisson-Dirac Neural Networks (PoDiNNs)

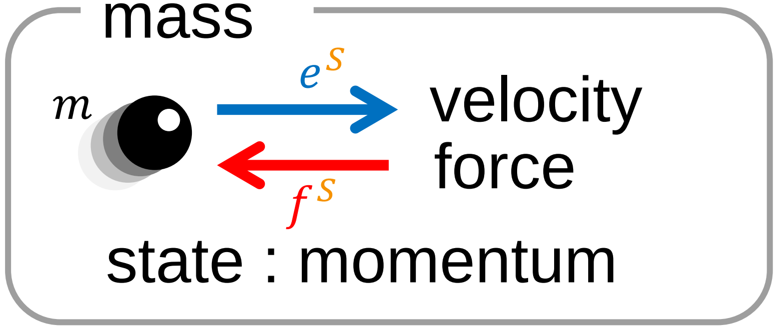
- as a unified way to model various aspect of physical phenomena.
- learn each component individually, then use Dirac structure to explicitly represent the coupling among components.

Proposed Method

Types of Components in PoDiNNs

- energy-storing components





inputs : flow $f = (f^S \ f^R \ f^I)$

outputs : effort $e = (e^S \ e^R \ e^I)$

^{S} : energy-storing components

Proposed Method

Types of Components in PoDiNNs

inputs : flow $f = (f^S \; f^R \; f^I)$

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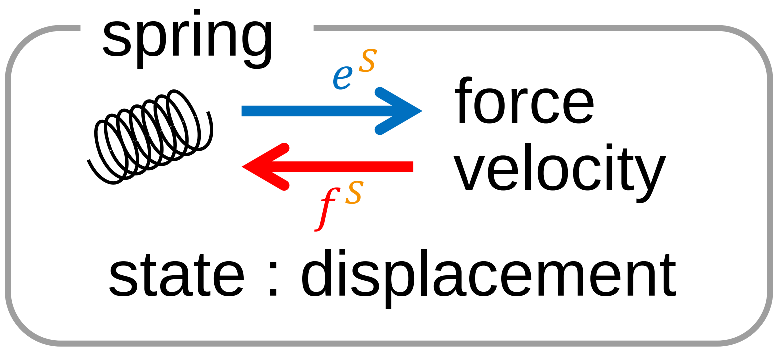
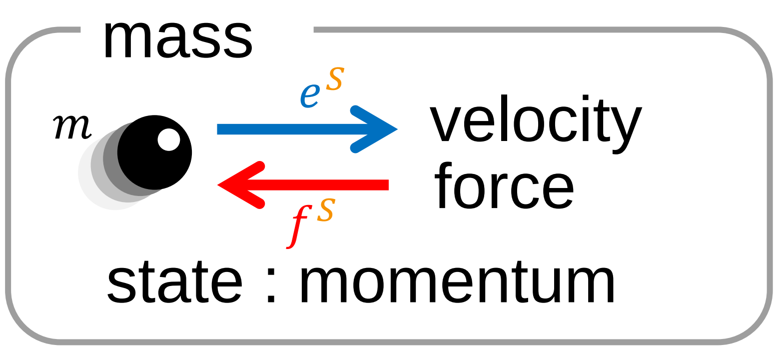
^{S} : energy-storing components

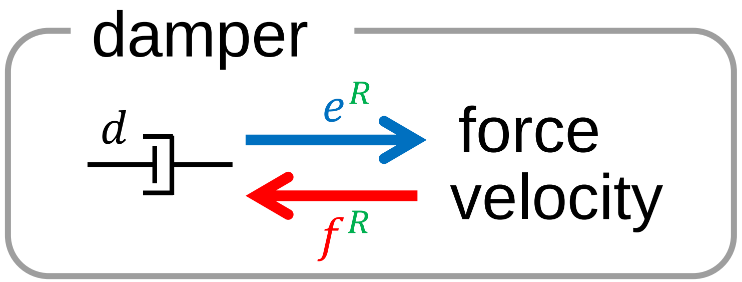
^{R} : energy-dissipating components

- energy-storing components





- energy-dissipating components



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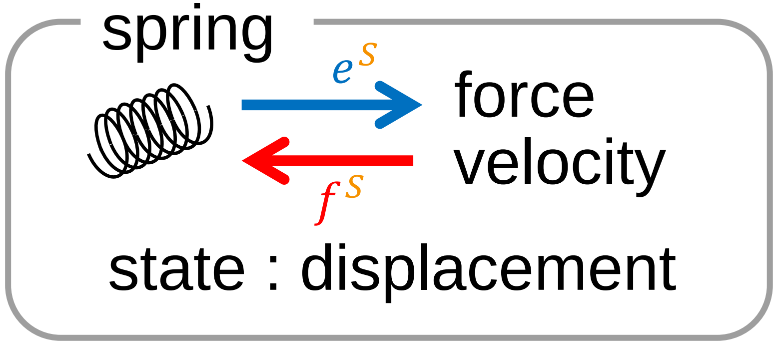
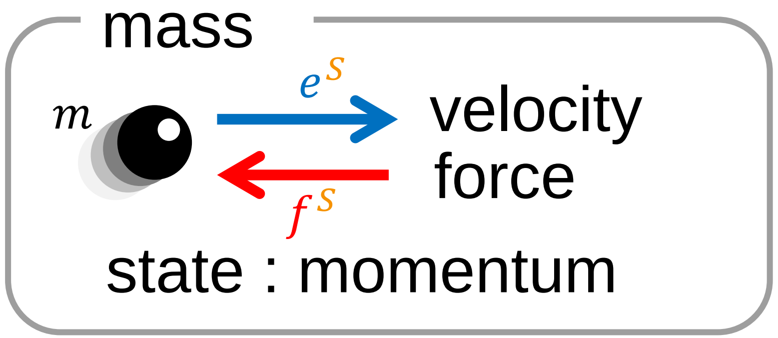
^{I} : external inputs

- energy-storing components





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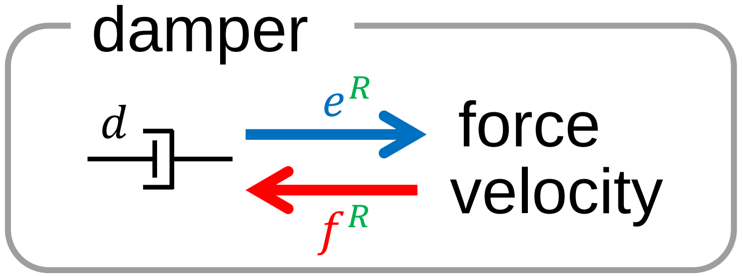
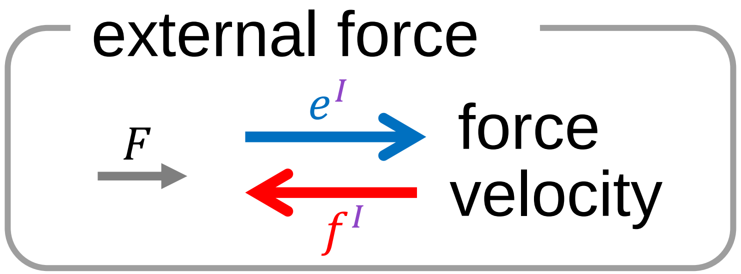


- external inputs



Proposed Method

Applicable to Various Physical Domains

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

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Proposed Method

Flow and Efforts

[5] van der Schaft+, 2014
[6] Duindam+, 2009

- We consider fibers $\mathcal{F}_{\boldsymbol{u}}$ and $\mathcal{E}_{\boldsymbol{u}}$ of the vector bundles $\mathcal{F}$ and $\mathcal{E} = \mathcal{F}^*$ at $\boldsymbol{u} \in \mathcal{M}$ which are decomposed as

$$\mathcal{F}_{\boldsymbol{u}} = \mathcal{F}_{\boldsymbol{u}}^S \oplus \mathcal{F}_{\boldsymbol{u}}^R \oplus \mathcal{F}_{\boldsymbol{u}}^I \text{ and } \mathcal{E}_{\boldsymbol{u}} = \mathcal{E}_{\boldsymbol{u}}^S \oplus \mathcal{E}_{\boldsymbol{u}}^R \oplus \mathcal{E}_{\boldsymbol{u}}^I,$$

where $\mathcal{F}_{\boldsymbol{u}}^S = T_{\boldsymbol{u}}\mathcal{M}$ and $\mathcal{E}_{\boldsymbol{u}}^S = T_{\boldsymbol{u}}^*\mathcal{M}$.

- A point on the fibers $\mathcal{F}_{\boldsymbol{u}}$ and $\mathcal{E}_{\boldsymbol{u}}$ is denoted by

$$\boldsymbol{f} = (\boldsymbol{f}^S, \boldsymbol{f}^R, \boldsymbol{f}^I) \text{ and } \boldsymbol{e} = (\boldsymbol{e}^S, \boldsymbol{e}^R, \boldsymbol{e}^I).$$

- We refer to $\boldsymbol{f} \in \mathcal{F}_{\boldsymbol{u}}$ as *flows*, $\boldsymbol{e} \in \mathcal{E}_{\boldsymbol{u}}$ as *efforts*, and both collectively as *port variables*.

Proposed Method

The Coupling of Flows and Efforts

Theorem

Consider vector bundles $\mathcal{F}$ and $\mathcal{E} = \mathcal{F}^*$ over manifold $\mathcal{M}$.

The collection of $D_{\boldsymbol{u}} = \left\{(\boldsymbol{f}, \boldsymbol{e}) \in \mathcal{F}_{\boldsymbol{u}} \oplus \mathcal{E}_{\boldsymbol{u}} \mid \boldsymbol{f} = B_{\boldsymbol{u}}^{\sharp}(\boldsymbol{e})\right\}$ for the bundle map $B_{\boldsymbol{u}}^{\sharp}: \mathcal{E}_{\boldsymbol{u}} \to \mathcal{F}_{\boldsymbol{u}}$ of a bivector B is a Dirac structure $D \subset \mathcal{F} \oplus \mathcal{E}$.

- This Dirac structure can reformulate Hamiltonian, Poisson, constrained Hamiltonian and port-Hamiltonian systems.

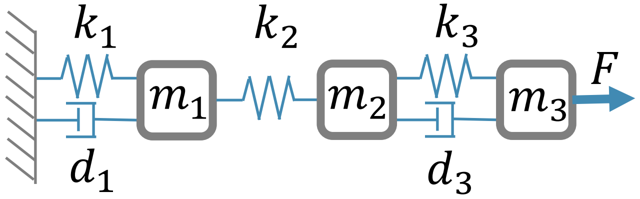
Proposed Method

Formulation

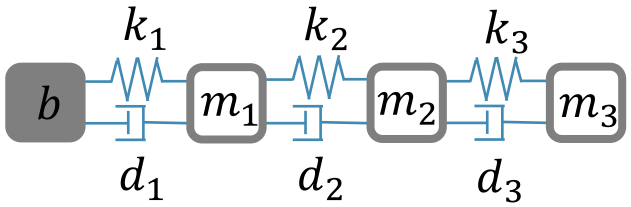
$$\begin{bmatrix} \boldsymbol{f}^S \\ \boldsymbol{f}^R \\ \boldsymbol{f}^I \end{bmatrix} = B_{\boldsymbol{u}}^{\sharp} \begin{bmatrix} \boldsymbol{e}^S \\ \boldsymbol{e}^R \\ \boldsymbol{e}^I \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} \dot{\boldsymbol{u}} \\ \boldsymbol{f}^R \\ \boldsymbol{f}^I \end{bmatrix} = B_{\boldsymbol{u}}^{\sharp} \begin{bmatrix} \nabla_{\boldsymbol{u}} H(\boldsymbol{u}) \\ R_{\boldsymbol{u}}(\boldsymbol{f}^R) \\ \boldsymbol{e}^I(t) \end{bmatrix}$$

- flow $\boldsymbol{f}^S$: time evolution $\dot{\boldsymbol{u}}$ of the state $\boldsymbol{u}$.
- effort $\boldsymbol{e}^S$: differential $\mathrm{d}H$ of the Hamiltonian H.
- effort $\boldsymbol{e}^R$: dissipative force determined by a mapping $R_{\boldsymbol{u}}\colon \boldsymbol{f}^R \mapsto \boldsymbol{e}^R$.
- effort $\boldsymbol{e}^I$: external input depending on time t.
- $H, R_{\boldsymbol{u}}$ and $B_{\boldsymbol{u}}^{\sharp}$ are learned using deep learning.

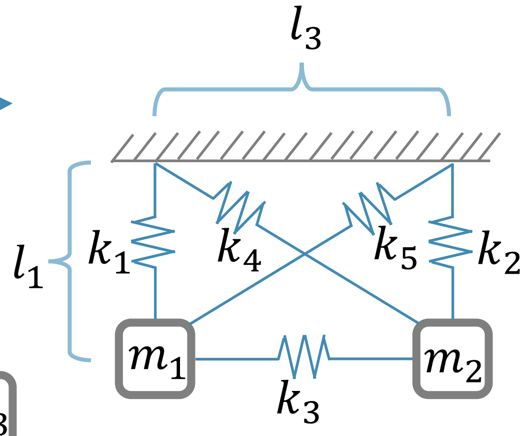
Experiments：Datasets



(a) with external force

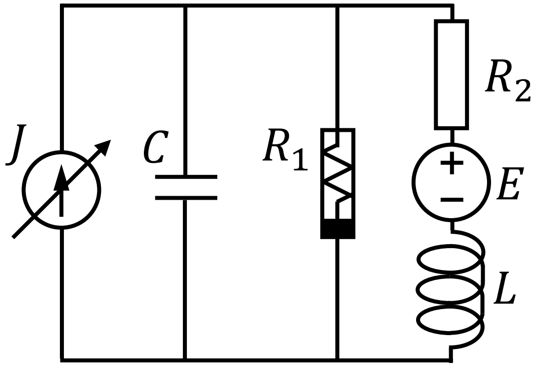


(b) with moving boundary

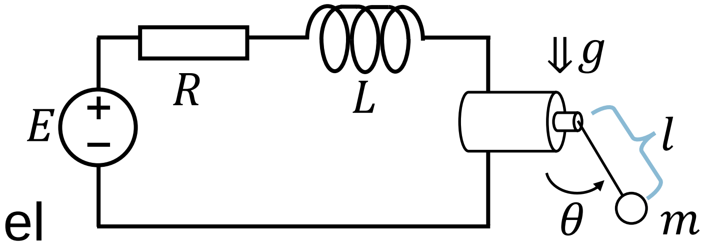


(c) with redundancy

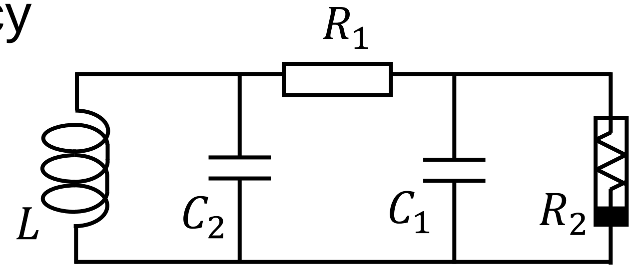
(a)-(c) Mass-spring(-damper) systems



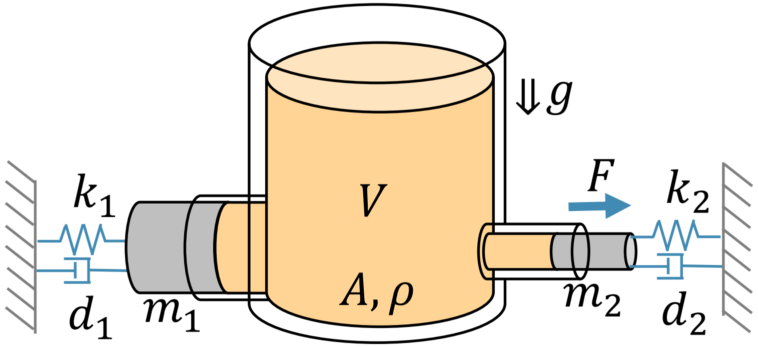
(d) FitzHugh-Nagumo model



(f) DC motor

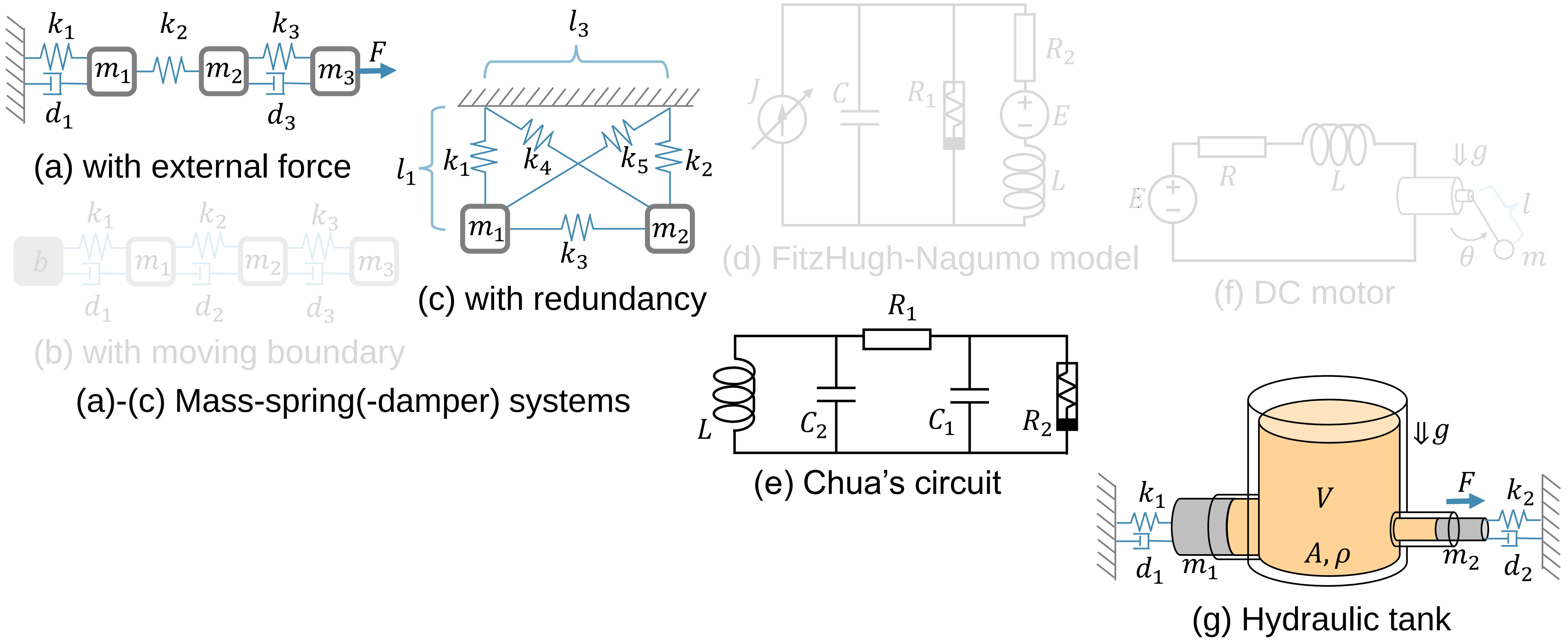


(e) Chua's circuit



(g) Hydraulic tank

Experiments：Datasets



(a)-(c) Mass-spring(-damper) systems

Experiments：Results

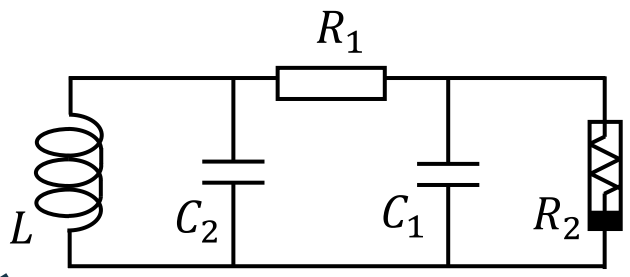
Dataset	Mass-Spring-Damper Systems			
	(a) with external force		(c) with redundancy	
Subdomain	MSE↓	VPT↑	MSE↓	VPT↑
Neural ODE	7.68 ± 1.07	0.097 ± 0.008	2490.61 ± 1847.24	0.099 ± 0.004
HNN Variants*	8.31 ± 0.56	0.104 ± 0.017	634.22 ± 300.01	0.000 ± 0.000
PoDiNN	$\mathbf{4.33} \pm 0.26$	$\mathbf{0.622} \pm 0.002$	$\mathbf{0.11} \pm 0.02$	$\mathbf{0.863} \pm 0.017$
	$\times 10^{-1}$	$\theta = 10^{-3}$	$\times 10^{-1}$	$\theta = 10^{-3}$

	Electric Circuits		Multiphysics	
	(e) Chua's		(g) Hydraulic Tank	
	MSE↓	VPT↑	MSE↓	VPT↑
Neural ODE	14.74 ± 1.33	0.287 ± 0.016	30.62 ± 8.22	0.045 ± 0.010
PoDiNN	$\mathbf{9.21} \pm 0.83$	$\mathbf{0.469} \pm 0.010$	$\mathbf{5.42} \pm 3.65$	$\mathbf{0.918} \pm 0.013$
	$\times 10^{-1}$	$\theta = 10^{-3}$	$\times 10^{-2}$	$\theta = 10^{-4}$

*Dissipative SymODENs for (a), and PNNs for (b)

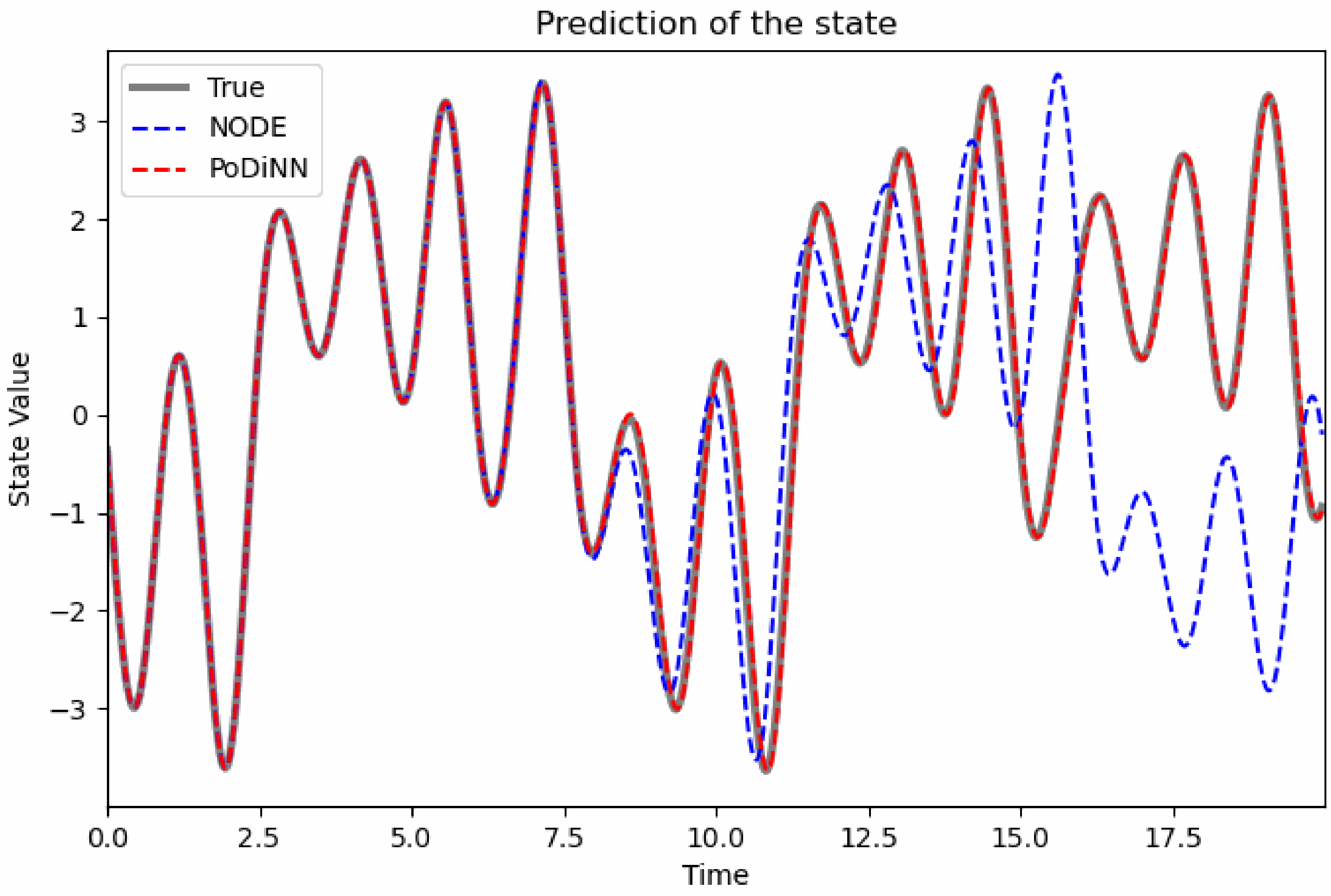
Experiments：Results

Visualization



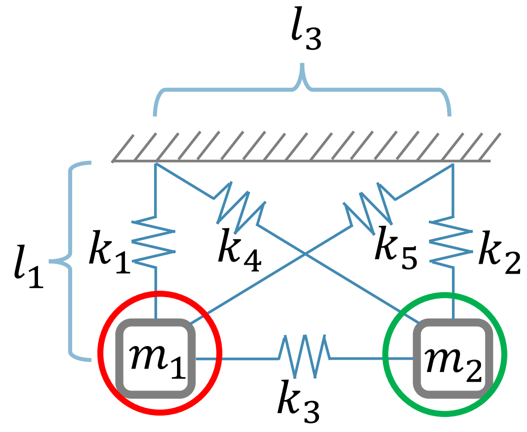
(e) Chua’s circuit

Predicting the current of the inductor



Experiments：Results

- PoDiNNs successfully learned the coupling patterns.



(b) Mass-spring system with redundancy

$$\dot{\boldsymbol{u}} = B_{\boldsymbol{u}}^{\sharp} \nabla_{\boldsymbol{u}} H(\boldsymbol{u})$$

submatrix of $B_{\boldsymbol{u}}^{\sharp}$

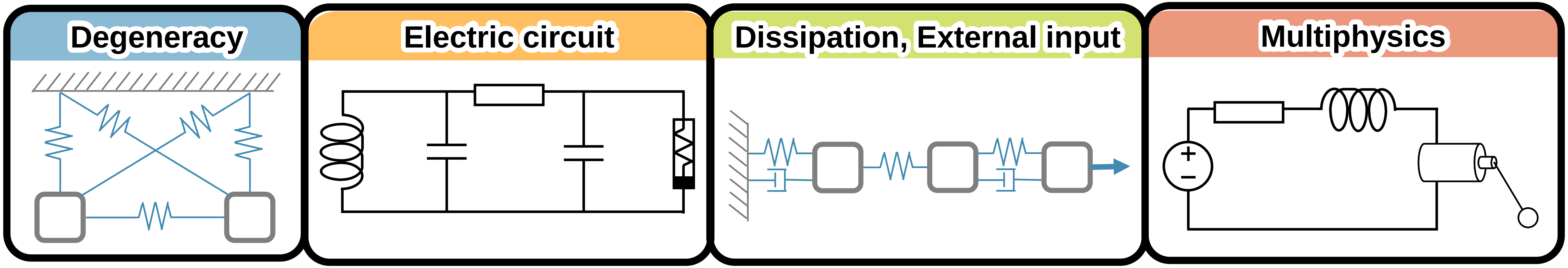
$$\begin{array}{c} \\ k_1 \\ \\ k_2 \\ \\ k_3 \\ \end{array} \overset{\qquad m_1 \qquad\qquad m_2}{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}}$$

This system has degeneracy !

$$Row(k_3) = Row(k_2) - Row(k_1)$$

Conclusion

We proposed PoDiNNs, a unified framework capable of handling various dynamical systems across multiple domains.



Through experiments, PoDiNNs

- achieved superior long-term prediction performance compared to existing methods.
- successfully identified the coupling patterns within the system.