On the use of thermodynamics biases for learning physical phenomena

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España | digital 2026

CALISTA workshop 2024

esi

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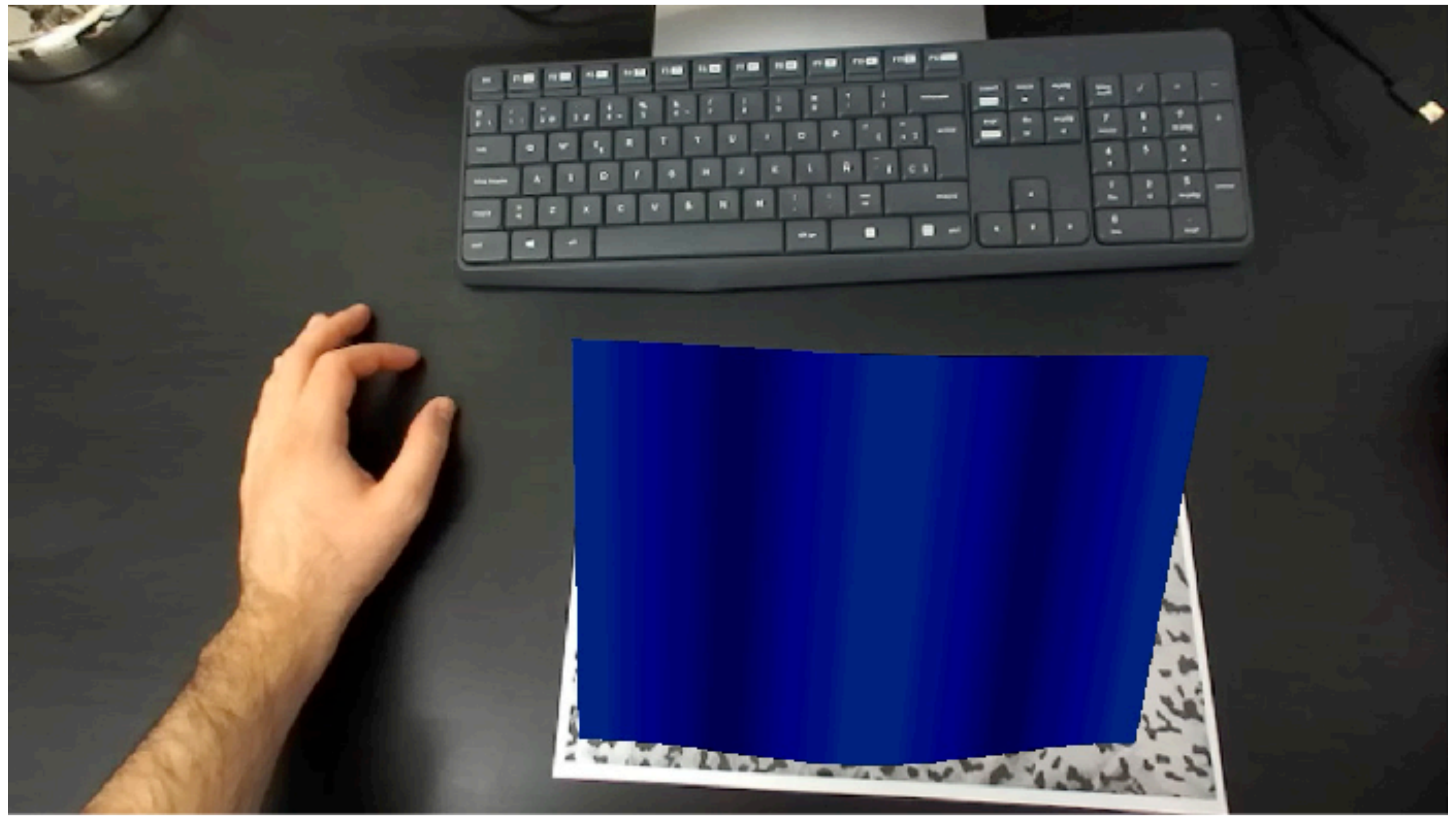
Motivation: world models

"Scientists […] need to build AI that doesn't just operate by matching patterns but can also reason about the physical world". [1]

"It's about modeling the world…" [2]

"… to create machines that can learn internal models of how the world works […], plan how to accomplish complex tasks, and readily adapt to unfamiliar situations." [3]

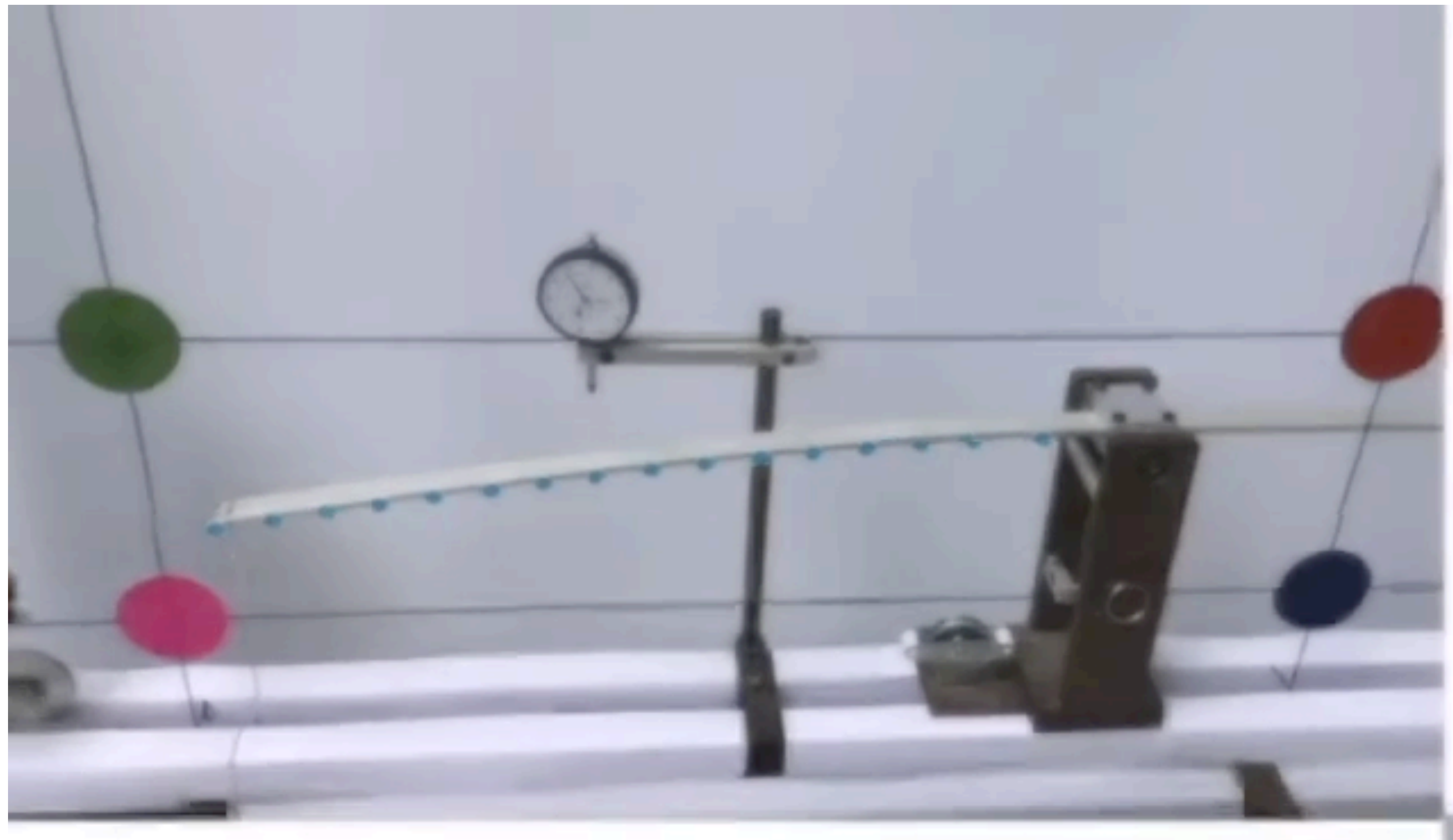


Badias, Alberto, et al. "Morph-DSLAM: Model order reduction for physics-based deformable SLAM." *IEEE Transactions on Pattern Analysis and Machine Intelligence* 44.11 (2021): 7764-7777.

[1]. Matthew Hutson, Nature Index, November 17th 2023.
[2]. Lake, B. M., Ullman, T. D., Tenenbaum, J. B., & Gershman, S. J. (2017). Building machines that learn and think like people. *Behavioral and brain sciences*, *40*, e253.
[3] LeCun, Y. (2022). A path towards autonomous machine intelligence version 0.9. 2, 2022-06-27. *Open Review*, *62*.

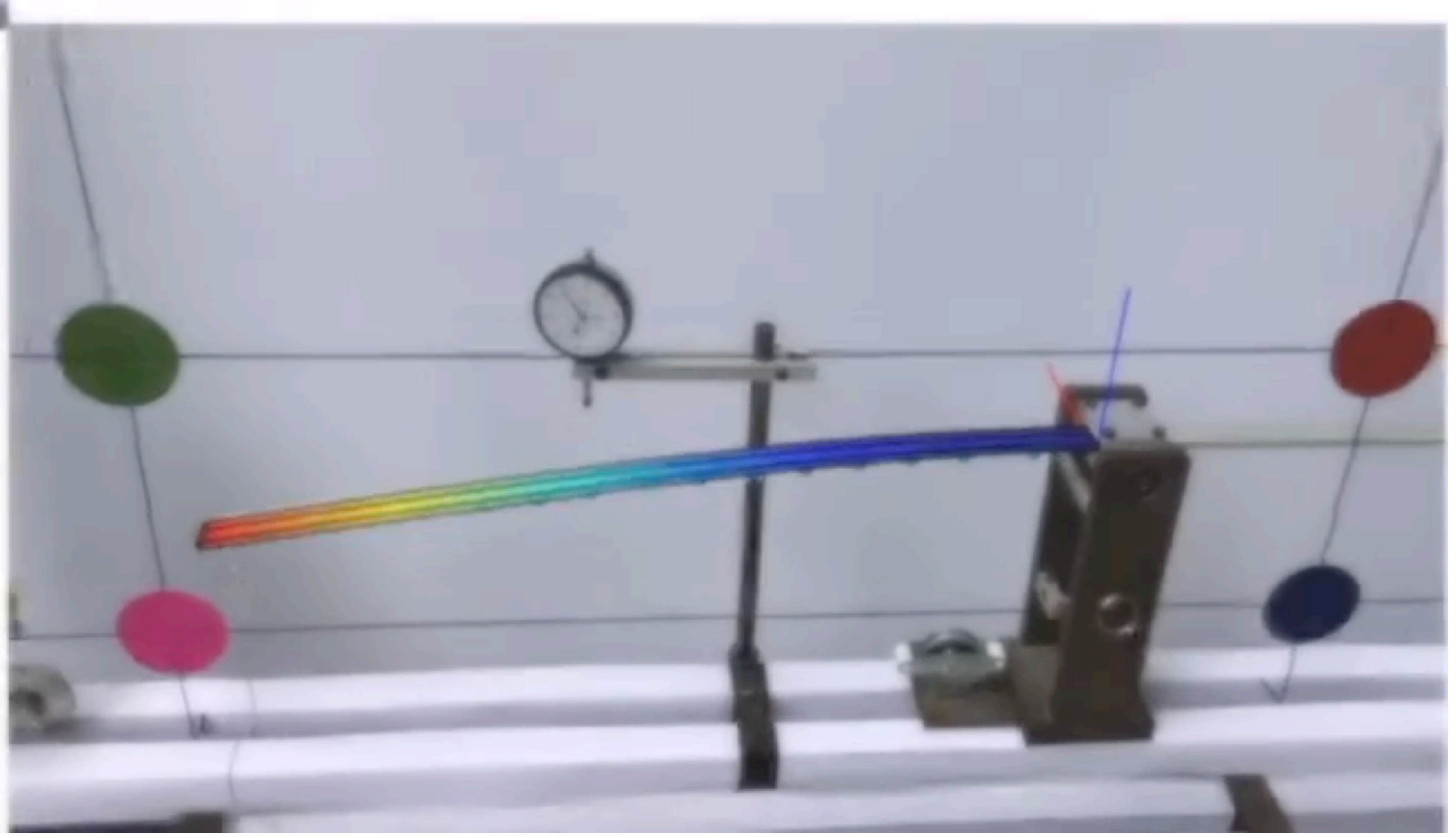
Cognitive digital twins

What the the AI “thinks”



What the camera sees

AR information to the user

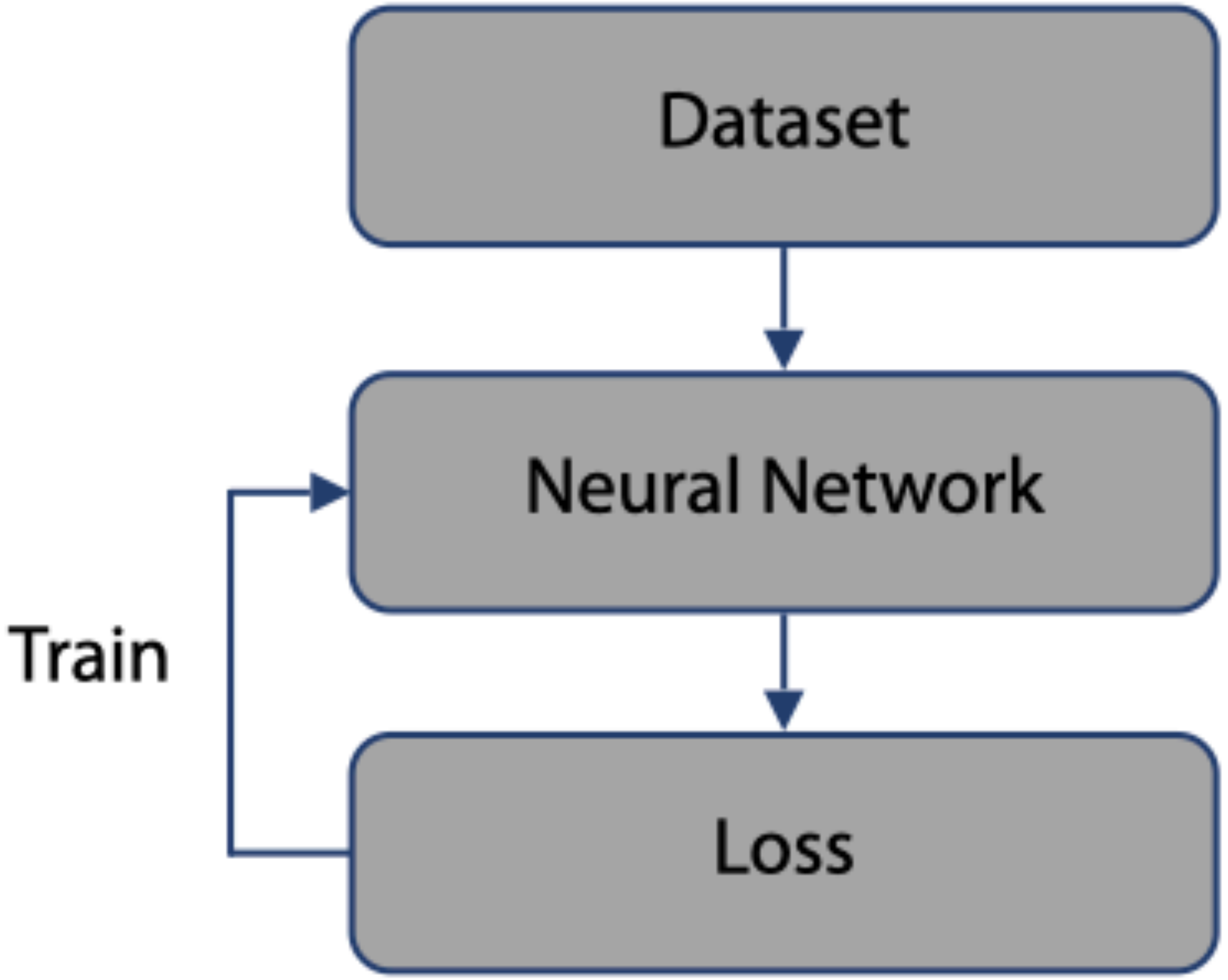


Our approach to digital twins

- Able to see (through computer vision)
- Able to understand what they see (perception, machine learning)
- Able to make prognosis (reasoning, real-time simulation)
- Able to inform for decision making (Augmented Reality)

Motivation: structured vs. unstructured approaches

- Scientific Deep Learning



Observational bias

Inductive bias

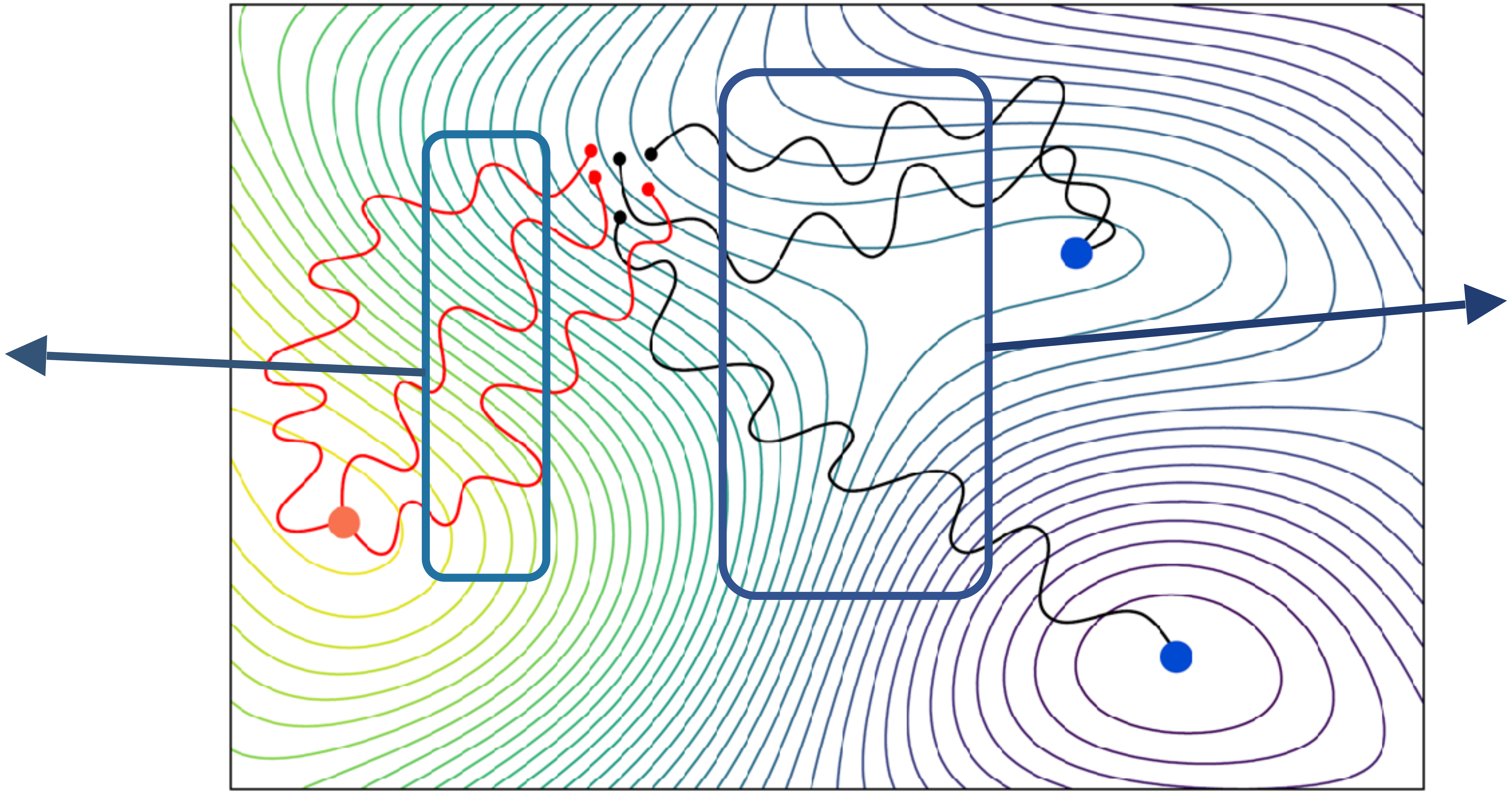
NeuralODE [Chen, 2018]
FNO [Li, 2020]
MP-GNN [Gilmer, 2017]
MeshGraphNet [Pfaff, 2020]

Learning bias

PINNs [Raissi, 2019]
DeepONet [Lu, 2019]

The importance of inductive biases

Loss landscape



Strong bias
Physics
+
Domain

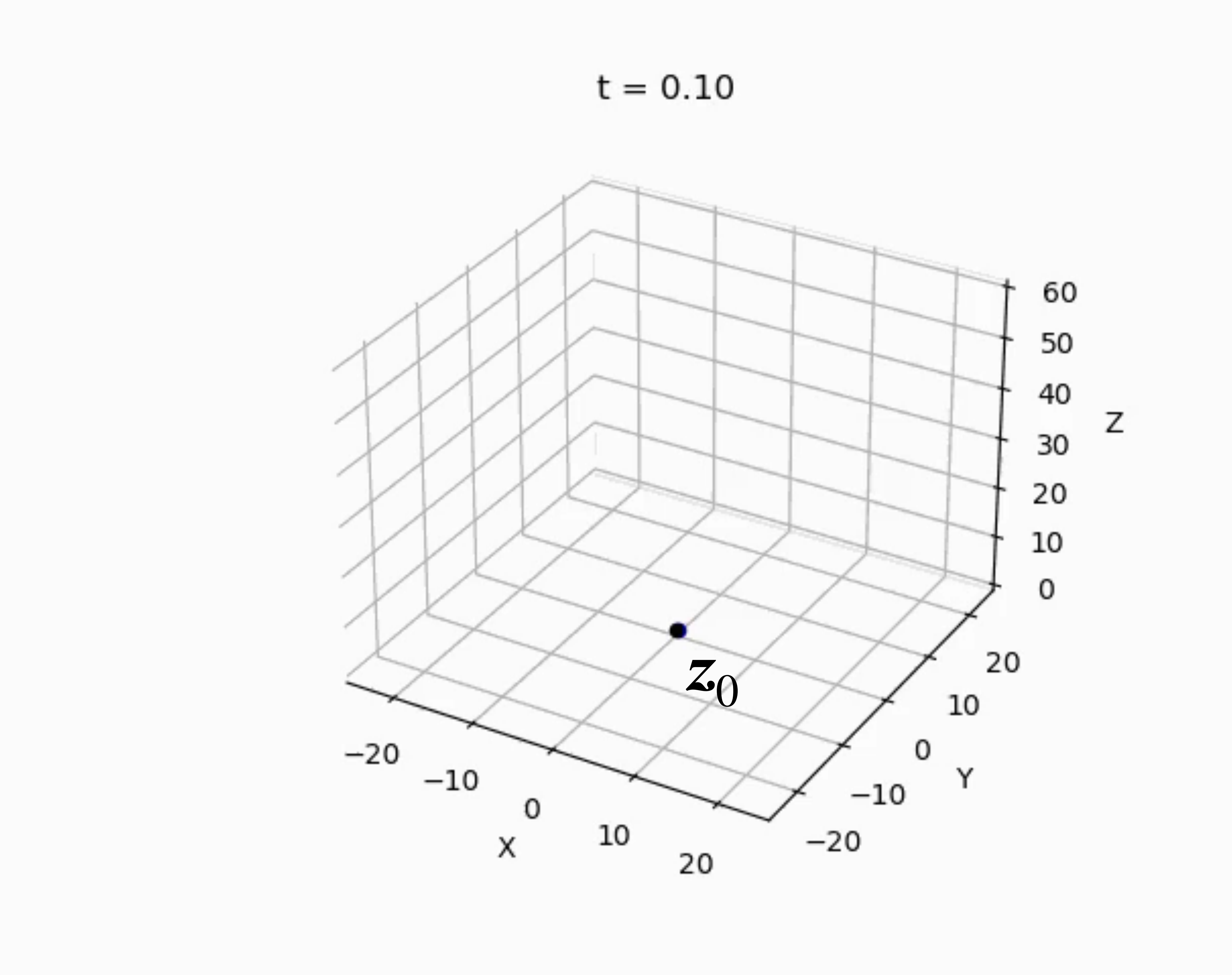
Weak bias

Problem statement

- Learn a dynamical system from data
- State vector: $\boldsymbol{z} = \left(z_1, z_2, \ldots\right)$

$$\dot{\boldsymbol{z}} = \frac{d\boldsymbol{z}}{dt} = \boxed{F(\boldsymbol{z}, t)}$$

- Time interval: $t \in (0,T]$
- Initial conditions: $\boldsymbol{z}(t=0) = \boldsymbol{z}_0$



Conservative systems, symmetries

- Hamiltonian mechanics
  - State variables: $\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p})$
  - Hamiltonian: $\mathscr{H} = \mathscr{H}(\boldsymbol{q}, \boldsymbol{p}) = T(\boldsymbol{p}) + V(\boldsymbol{q})$

Hamilton's equations

$$\begin{cases} \dfrac{d\boldsymbol{p}}{dt} = -\dfrac{\partial \mathscr{H}}{\partial \boldsymbol{q}} \\[2ex] \dfrac{d\boldsymbol{q}}{dt} = \dfrac{\partial \mathscr{H}}{\partial \boldsymbol{p}} \end{cases} \longrightarrow \begin{pmatrix} \dfrac{dq}{dt} \\[1ex] \dfrac{dp}{dt} \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & \boldsymbol{1} \\ -\boldsymbol{1} & 0 \end{pmatrix}}_{\boldsymbol{L}(\boldsymbol{z})} \begin{pmatrix} \dfrac{\partial \mathscr{H}}{\partial q} \\[1ex] \dfrac{\partial \mathscr{H}}{\partial p} \end{pmatrix}$$

- Poisson matrix
- Skew-symm

$$\frac{d\boldsymbol{z}}{dt} = \boldsymbol{L}\frac{\partial E}{\partial \boldsymbol{z}}$$

- Symplectic
- Reversible

Conservative systems, symmetries

- Hamiltonian mechanics
  - State variables: $\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p})$
  - Hamiltonian: $\mathscr{H} = \mathscr{H}(\boldsymbol{q}, \boldsymbol{p}) = T(\boldsymbol{p}) + V(\boldsymbol{q})$

Hamilton's equations

$$\begin{cases} \dfrac{d\boldsymbol{p}}{dt} = -\dfrac{\partial \mathscr{H}}{\partial \boldsymbol{q}} \\[2ex] \dfrac{d\boldsymbol{q}}{dt} = \dfrac{\partial \mathscr{H}}{\partial \boldsymbol{p}} \end{cases}$$

Hamiltonian NN [Sánchez-González, 2019]
SympNets [Jin, 2020]
Lagrangian NN [Bhatoo, 2021]
Poisson NN [Jin, 2023]

$$\frac{d\boldsymbol{z}}{dt} = \boldsymbol{L}\frac{\partial E}{\partial \boldsymbol{z}}$$

- Symplectic
- Reversible

Dissipative systems: one-generator formalism

- Generalized Onsager formalism:

$$\dot{\boldsymbol{z}} = -\left(\boldsymbol{L}(\boldsymbol{z}) + \boldsymbol{M}(\boldsymbol{z})\right)\frac{\partial \mathcal{F}}{\partial \boldsymbol{z}},$$

- $\boldsymbol{L}$ is a skew-symmetric (Poisson) matrix and $\boldsymbol{M}$ a symmetric, positive semi-definite matrix

- $\mathcal{F}$ is a free-energy potential.

Yu, H., Tian, X., Weinan, E., & Li, Q. (2021). OnsagerNet: Learning stable and interpretable dynamics using a generalized Onsager principle. *Physical Review Fluids*, *6*(11), 114402.

Dissipative systems: two-generator GENERIC formalism

- The generalized free energy is assumed to take the form

$$\mathcal{F} = E + S$$

- So that

$$\dot{\boldsymbol{z}} = \boldsymbol{L}(\boldsymbol{z})\frac{\partial E}{\partial \boldsymbol{z}} + \boldsymbol{M}(\boldsymbol{z})\frac{\partial S}{\partial \boldsymbol{z}}, \longrightarrow \dot{\boldsymbol{z}} = \{\boldsymbol{z}, E\} + [\boldsymbol{z}, S]$$

- with the additional (degeneracy) conditions

$$\boldsymbol{L}(\boldsymbol{z})\frac{\partial S}{\partial \boldsymbol{z}} = \boldsymbol{0}, \qquad \boldsymbol{M}(\boldsymbol{z})\frac{\partial E}{\partial \boldsymbol{z}} = \boldsymbol{0}$$

- ensures the fulfillment of the 1st and 2nd principles of thermodynamics

González, D., Chinesta, F., & Cueto, E. (2019). Thermodynamically consistent data-driven computational mechanics. *Continuum Mechanics and Thermodynamics*, *31*, 239-253.

One- vs. two-generator formalisms

- *“[Structured] methods have the advantage that the learned models have pre-determined structures and stability may be automatically ensured.”*
- But they *“may have the limitation that the structures imposed may be too restrictive to handle complex problems beyond benchmark examples."*

Expresiveness vs. learnability

Yu, H., Tian, X., Weinan, E., & Li, Q. (2021). OnsagerNet: Learning stable and interpretable dynamics using a generalized Onsager principle. *Physical Review Fluids*, *6*(11), 114402.

Structure-preserving neural networks

- Parametrization of GENERIC operators:

$$\boldsymbol{L} = \boldsymbol{l} - \boldsymbol{l}^{\top}, \qquad \boldsymbol{M} = \boldsymbol{m}\boldsymbol{m}^{\top}.$$

- Data loss:

$$\mathcal{L}_n^{\text{data}} = \left\| \frac{d\boldsymbol{z}^{\text{GT}}}{dt} - \frac{d\boldsymbol{z}^{\text{net}}}{dt} \right\|_2^2,$$

- Degeneracy loss:

$$\mathcal{L}_n^{\text{deg}} = \left\| \boldsymbol{L}\frac{\partial S}{\partial \boldsymbol{z}_n} \right\|_2^2 + \left\| \boldsymbol{M}\frac{\partial E}{\partial \boldsymbol{z}_n} \right\|_2^2.$$

- Global loss:

$$\mathcal{L} = \frac{1}{N_{\text{batch}}} \sum_{n=0}^{N_{\text{batch}}} (\lambda \mathcal{L}_n^{\text{data}} + \mathcal{L}_n^{\text{deg}}).$$

- Hernández, Q., Badías, A., González, D., Chinesta, F., & Cueto, E. (2021). Structure-preserving neural networks. *Journal of Computational Physics*, *426*, 109950. SOFT
- Lee, K., Trask, N., & Stinis, P. (2021). Machine learning structure preserving brackets for forecasting irreversible processes. *Advances in Neural Information Processing Systems*, *34*, 5696-5707. HARD
- Zhang, Z., Shin, Y., & Em Karniadakis, G. (2022). GFINNs: GENERIC formalism informed neural networks for deterministic and stochastic dynamical systems. *Philosophical Transactions of the Royal Society A*, *380*(2229), 20210207. HARD

Hard vs. soft imposition of structure

- *"… somewhat surprisingly, we observed that imposing soft constraints instead of hard ones yields even better results, while being far less computationally demanding."*

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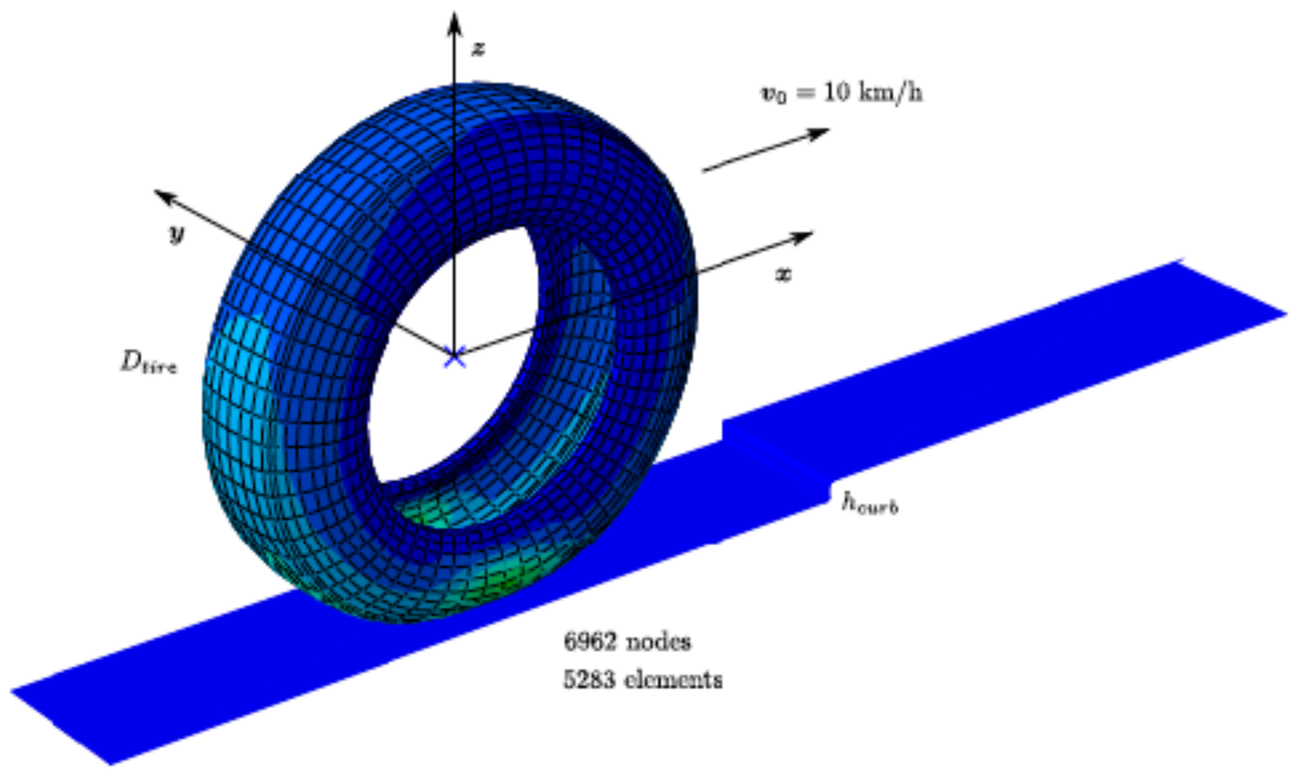
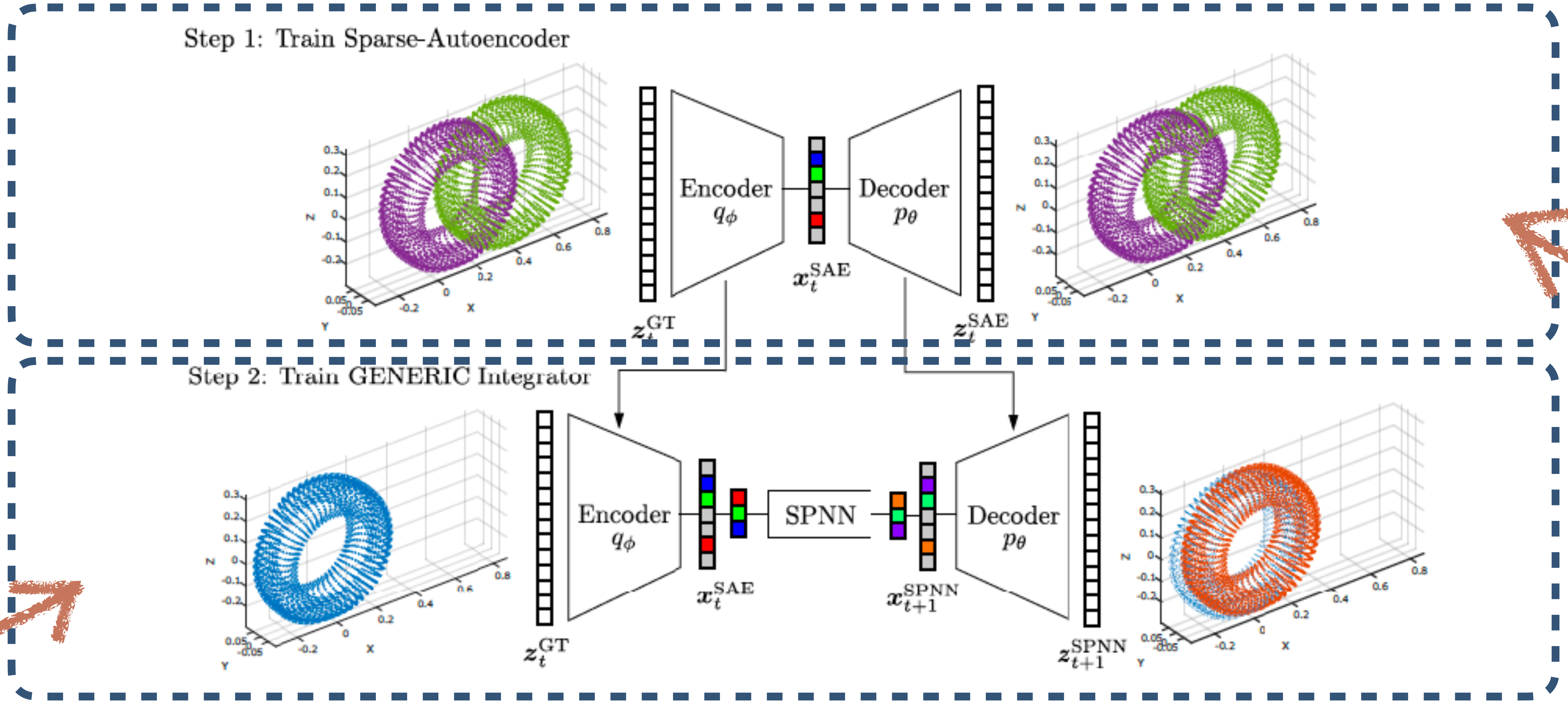
Márquez-Neila, P., Salzmann, M., & Fua, P. (2017). Imposing hard constraints on deep networks: Promises and limitations. *CVPR Workshop on Negative Results in Computer Vision, Hawaii, HI, 2017*

Structure-preserving ROMs

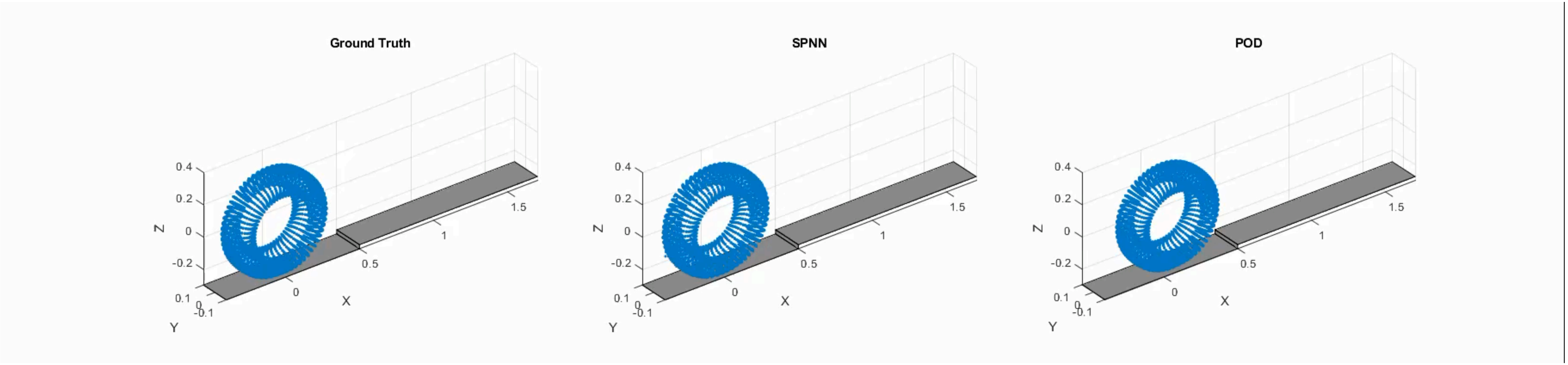


Unveil the intrinsic dimensionality of the manifold—L1 autoencoder

Structure-preserving time integration

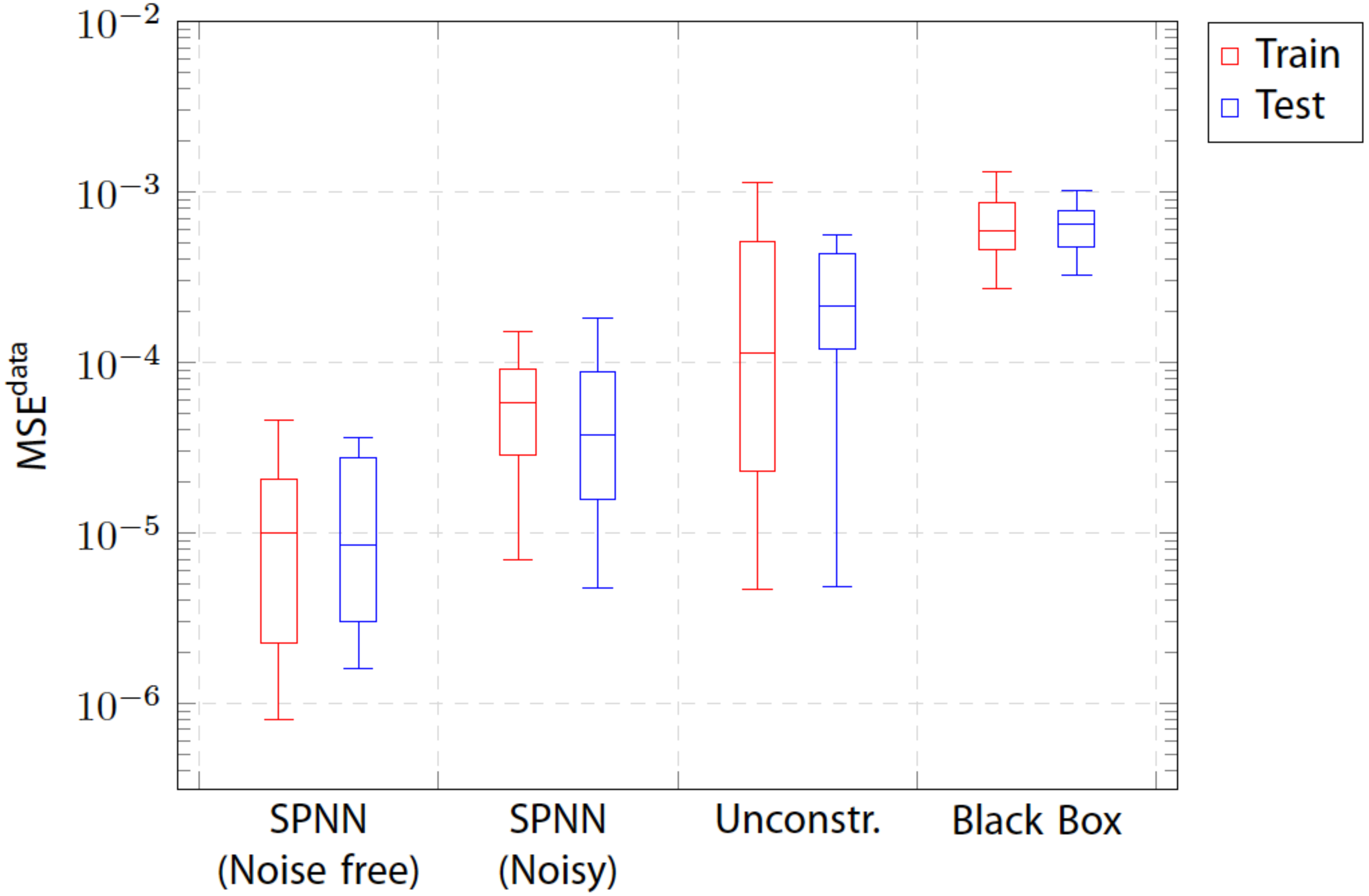


Results



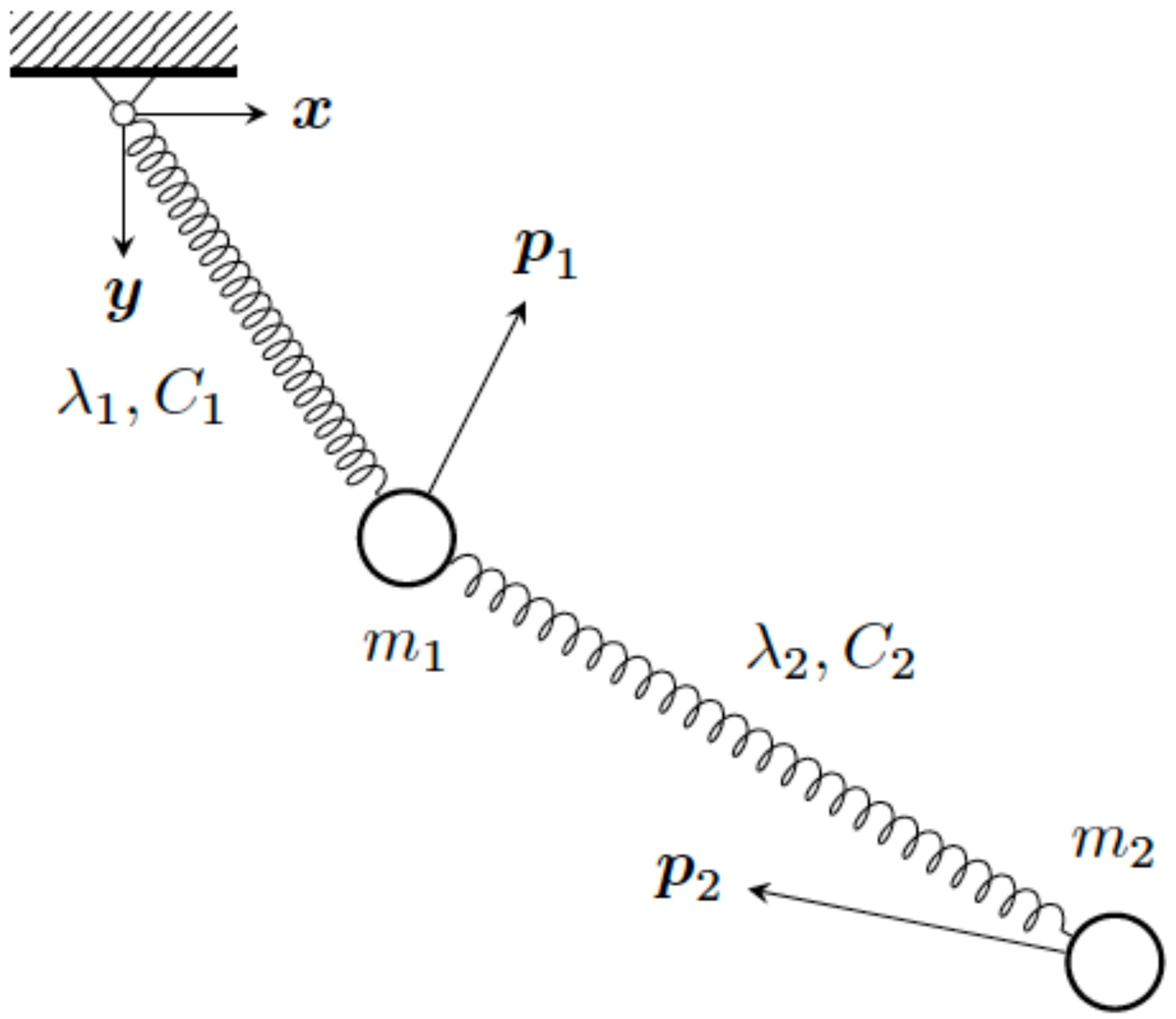
Hernandez, Q., Badias, A., Gonzalez, D., Chinesta, F., & Cueto, E. (2021). Deep learning of thermodynamics-aware reduced-order models from data. *Computer Methods in Applied Mechanics and Engineering*, *379*, 113763.

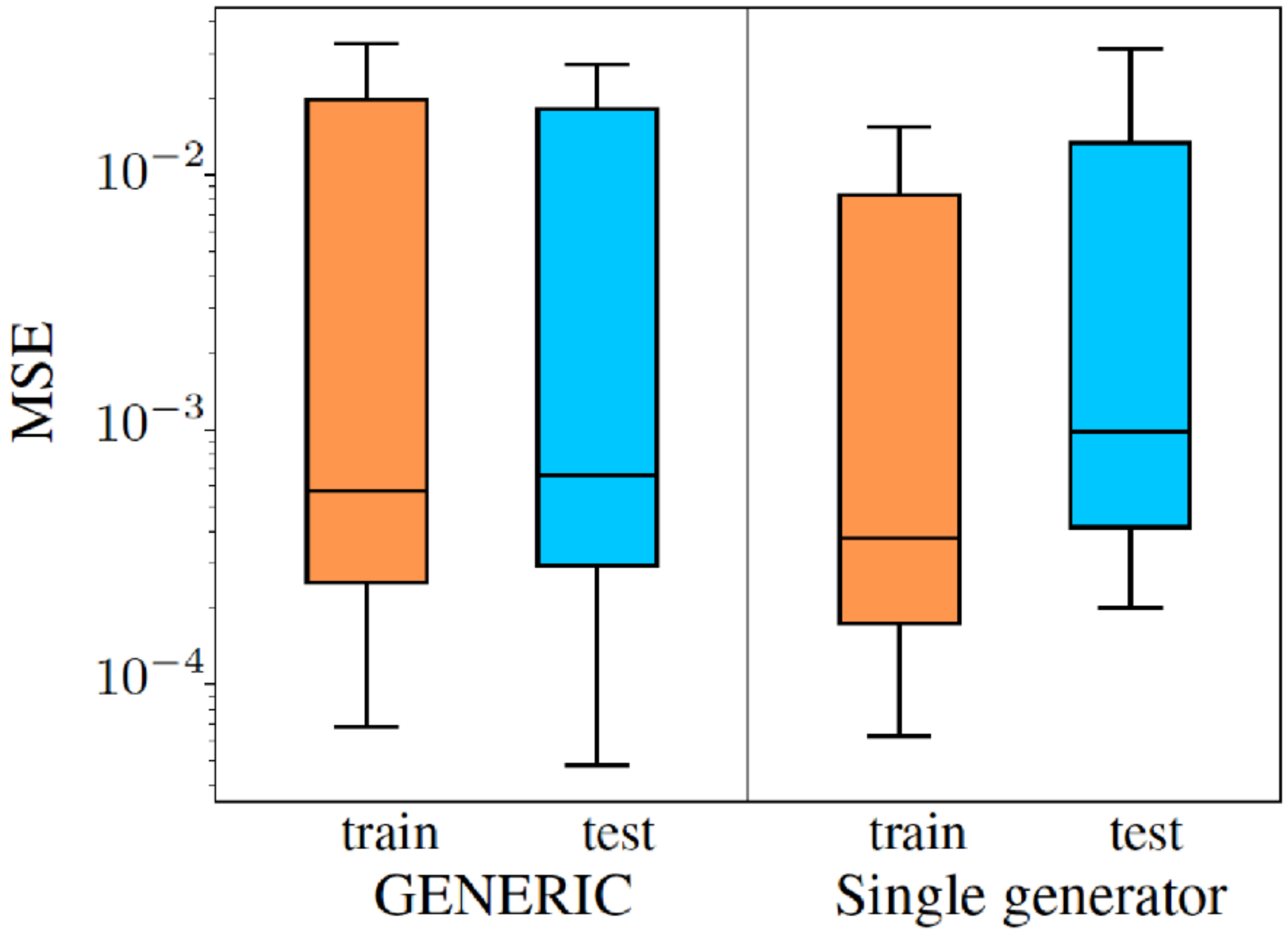
Take-home message



Hernández, Q., Badías, A., González, D., Chinesta, F., & Cueto, E. (2021). Structure-preserving neural networks. *Journal of Computational Physics*, *426*, 109950.

Comparison: Double thermoelastic pendulum





Urdeitx, P., Alfaro, I., González, D., Chinesta, F., & Cueto, E. (2024). A comparison of Single-and Double-generator formalisms for Thermodynamics-Informed Neural Networks. *arXiv preprint arXiv:2404.01060*.

Contents

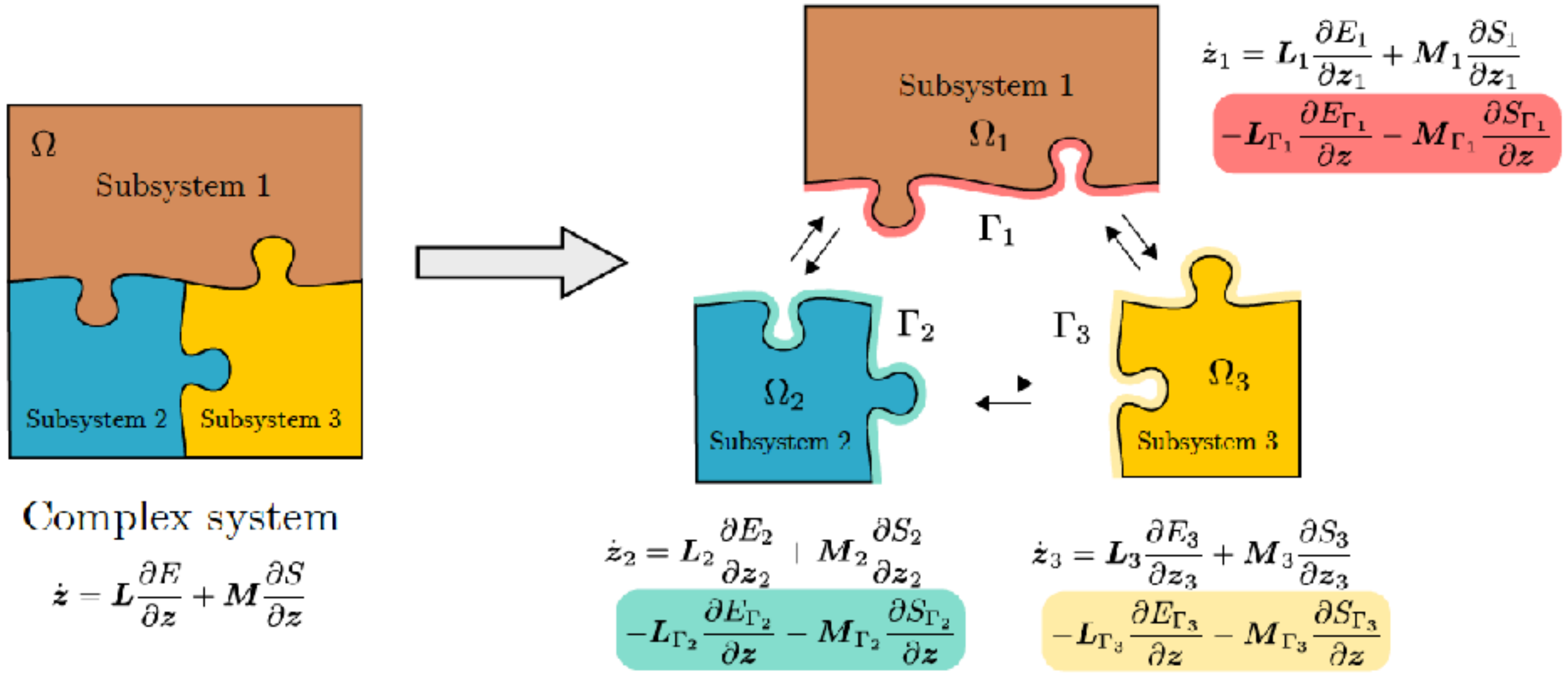
1. Metriplectic formalisms for open systems
2. Non-parametric domains

A port-metriplectic approach to learning

- Open systems:

$$\{\cdot,\cdot\} = \{\cdot,\cdot\}_{\text{bulk}} + \{\cdot,\cdot\}_{\text{boun}},$$

$$[\cdot,\cdot] = [\cdot,\cdot]_{\text{bulk}} + [\cdot,\cdot]_{\text{boun}}.$$

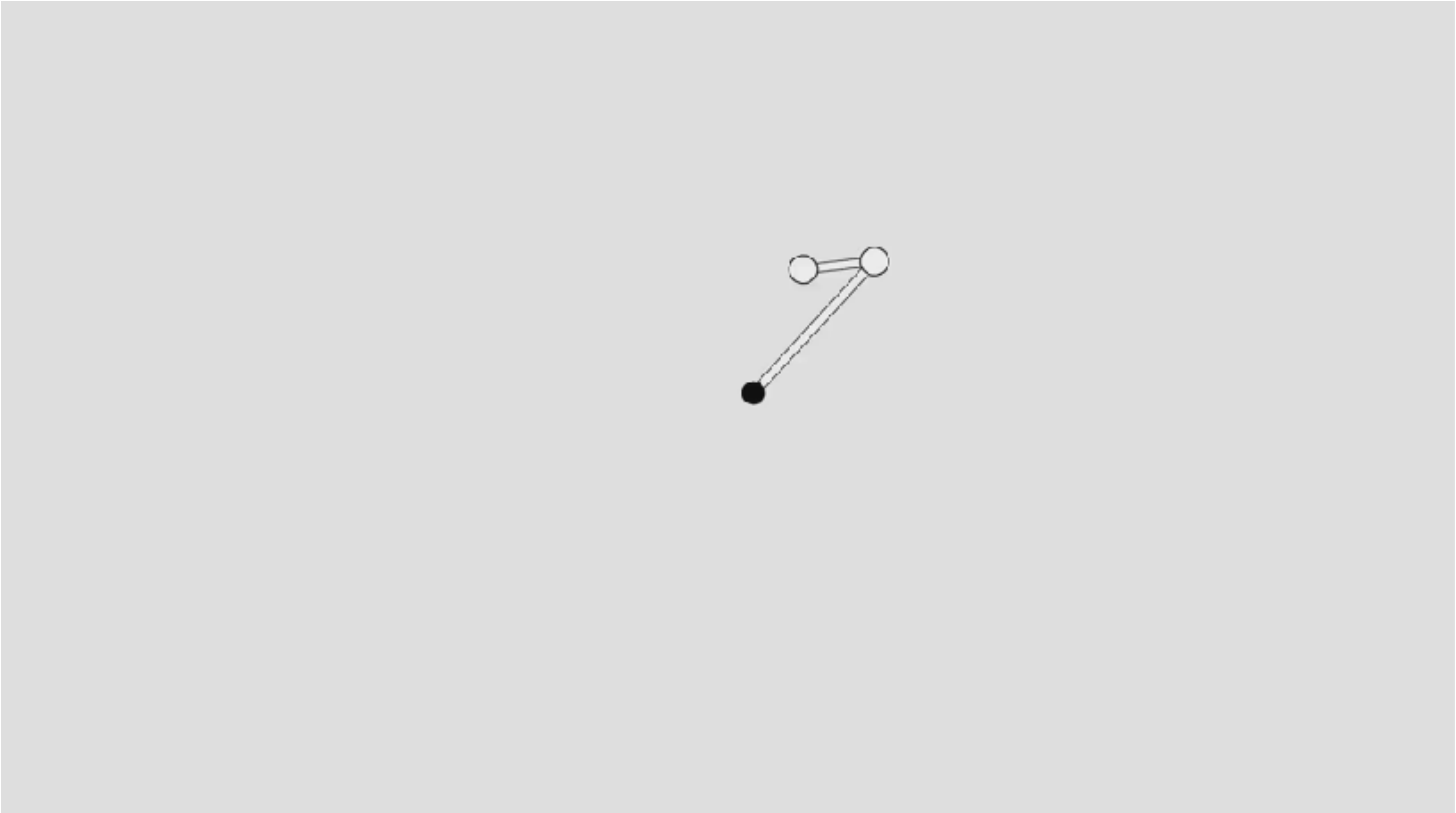


- Evolution of the open system:

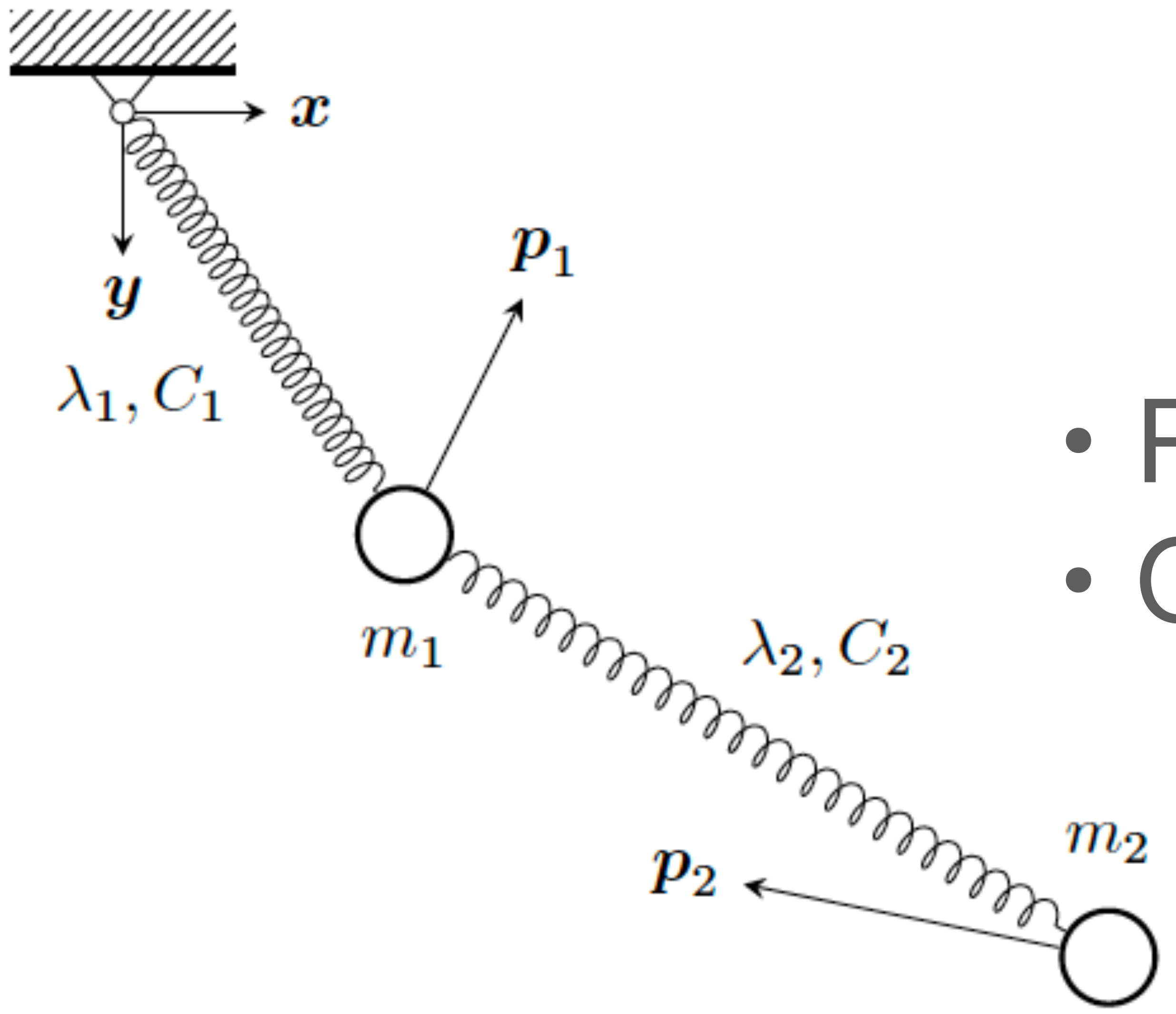
$$\dot{z} = \{z, E\}_{\text{bulk}} + [z, S]_{\text{bulk}}$$
$$= \{z, E\} + [z, S] - \{z, E\}_{\text{boun}} - [z, S]_{\text{boun}}.$$

- This generalizes the port-Metriplectic formalism
- Guarantees the right thermodynamic structure

Example: double thermoelastic pendulum



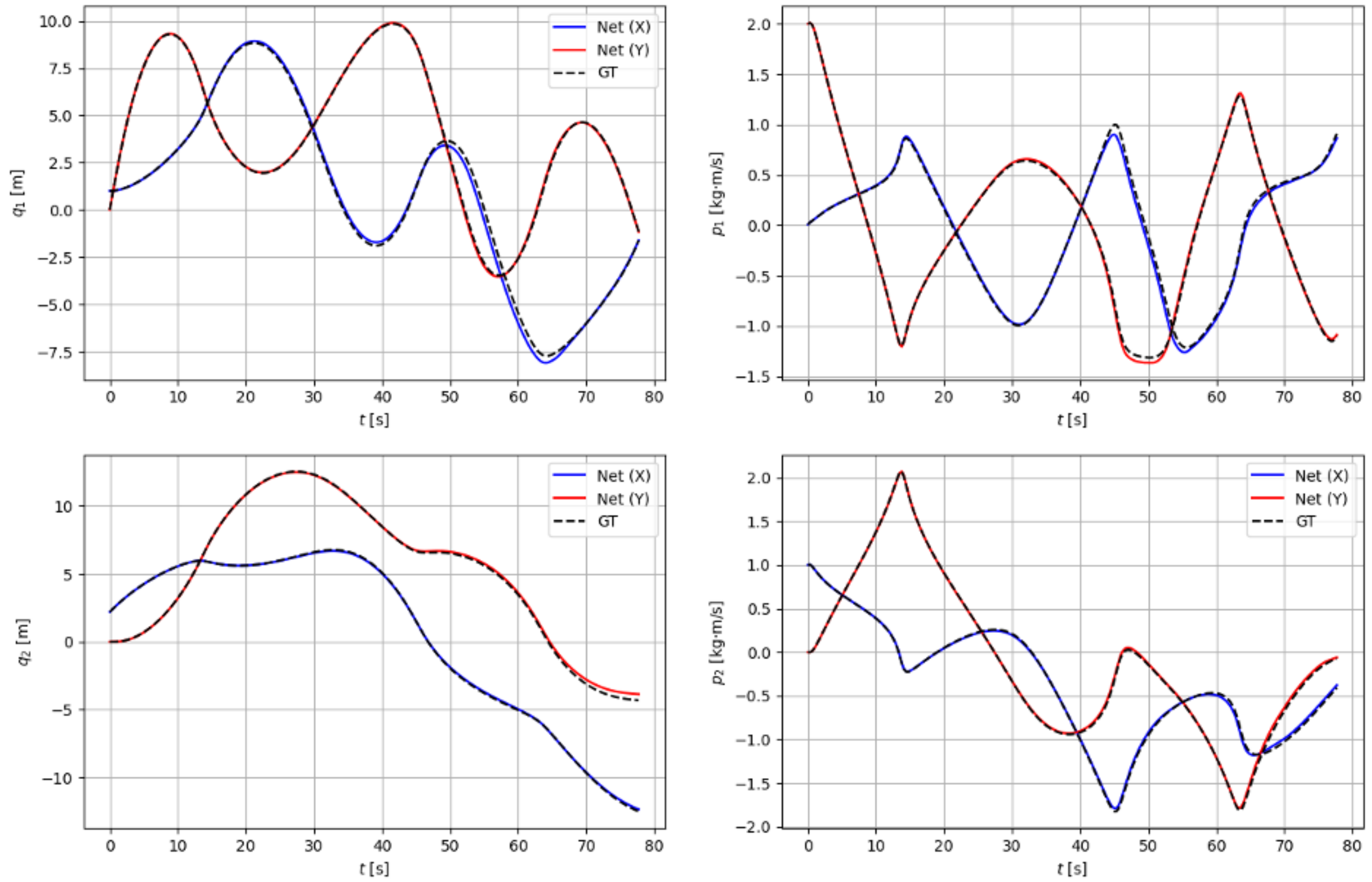
$$\mathcal{S} = \{\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p}, s) \in (\mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R})\}.$$



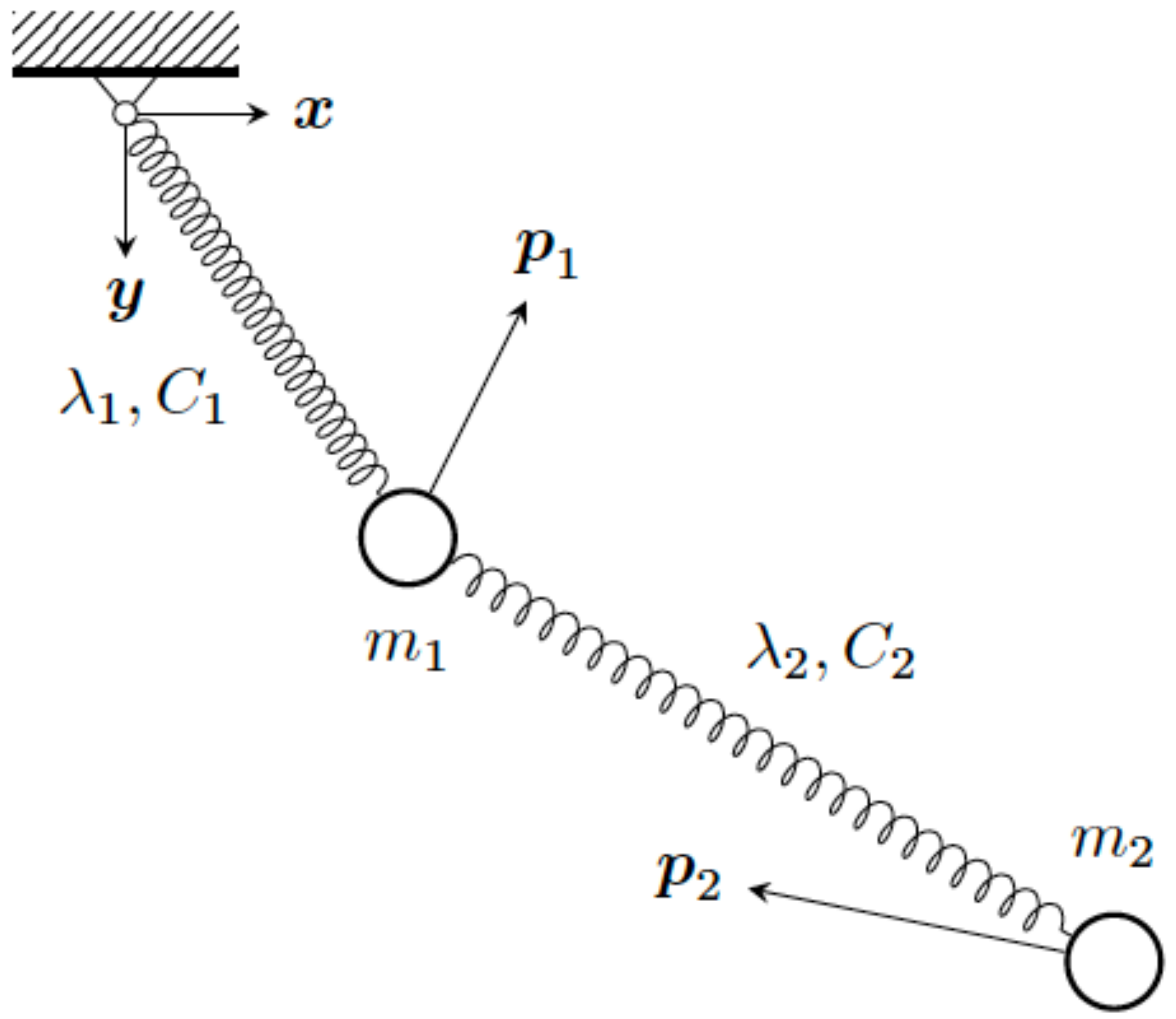
- Run 2x5 dof models
- Or 1x10 dof model

Hernández, Q., Badías, A., Chinesta, F., & Cueto, E. (2023). Port-metriplectic neural networks: thermodynamics-informed machine learning of complex physical systems. *Computational Mechanics*, 1-9.

Example: double thermoelastic pendulum

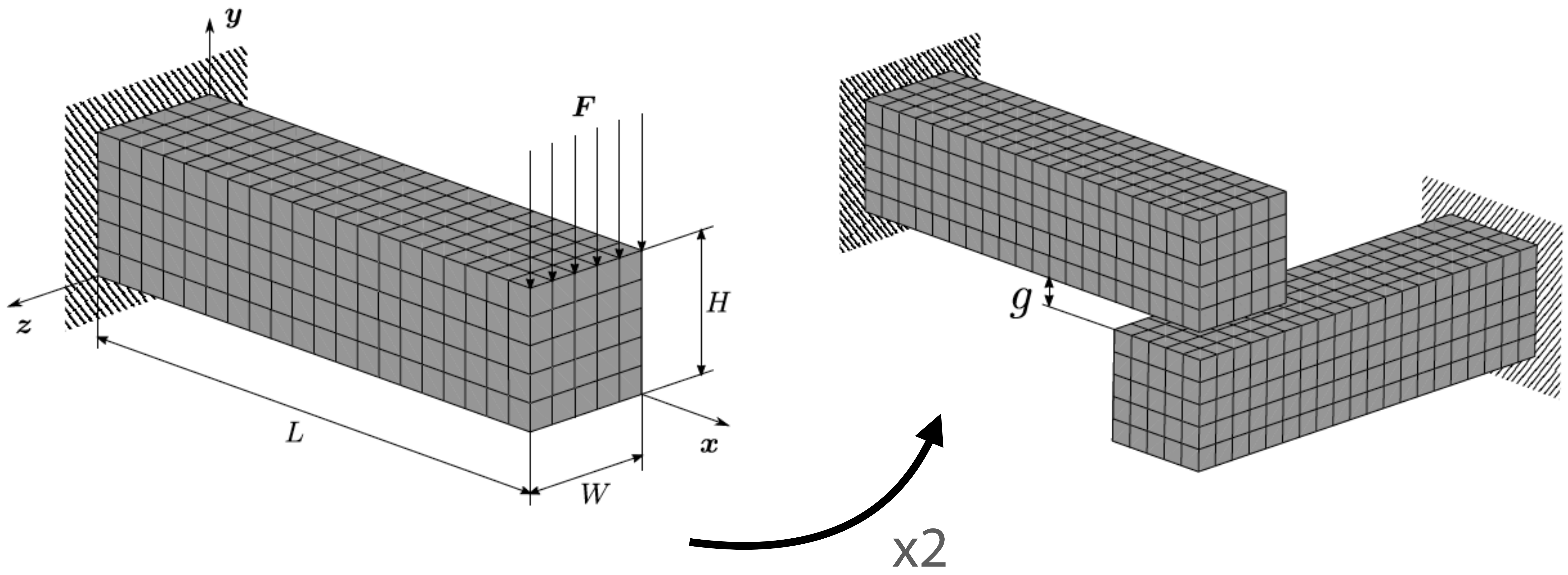


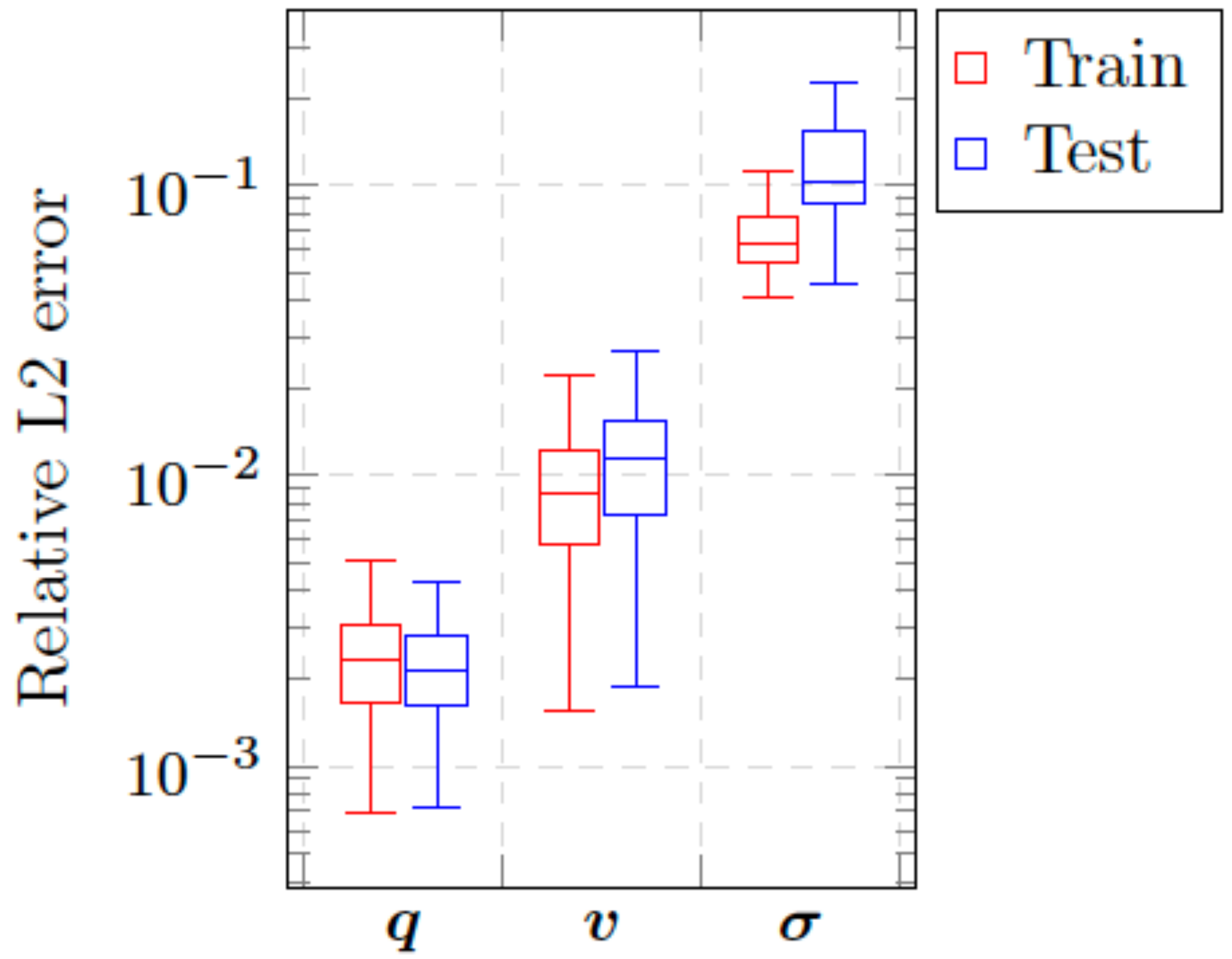
- Dataset with 50 trajectories with different initial conditions
- Split between train (80%) + test (20%) database



Viscous-hyperelastic beams interacting

- GNNs
- We learn one, the model contains two



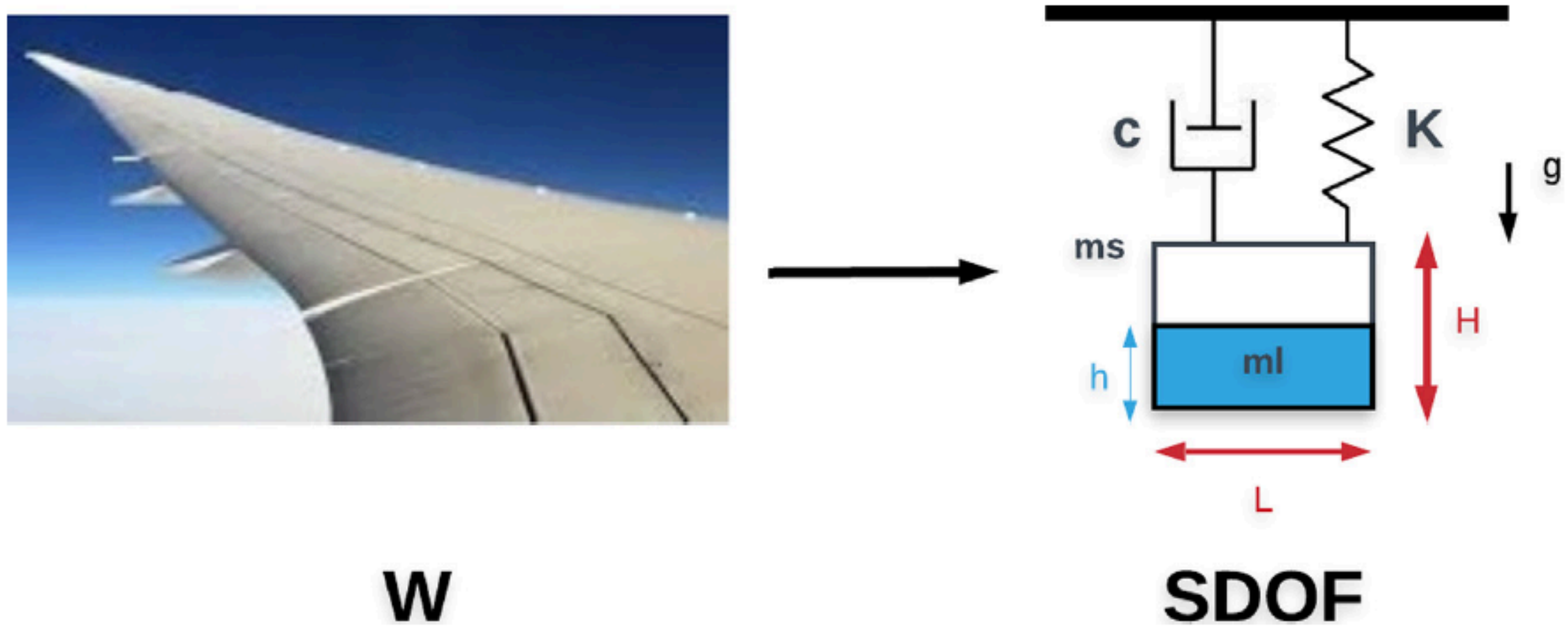


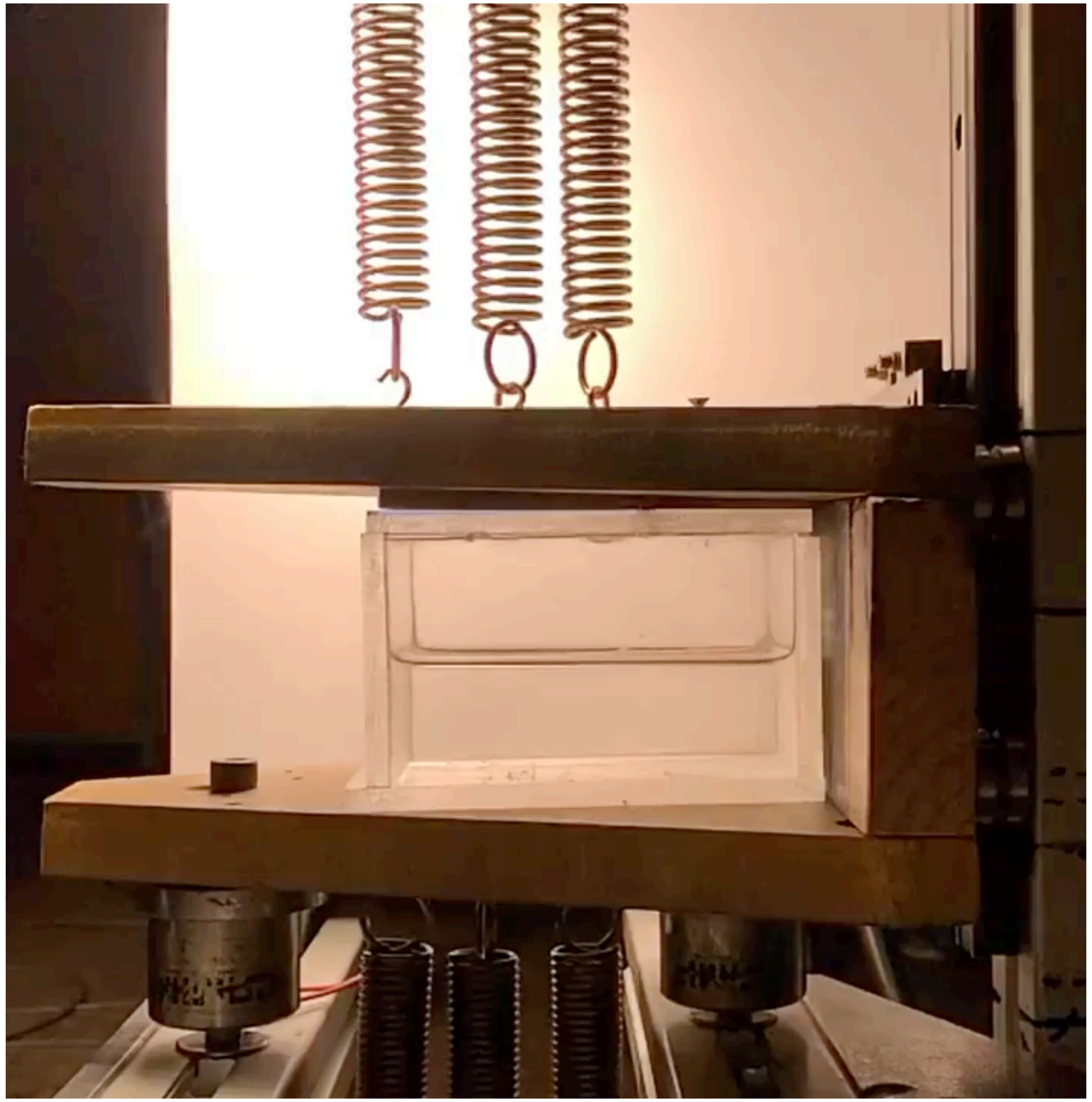
Viscous-hyperelastic beams interacting (Mixed Reality)

Hernández, Q., Badías, A., Chinesta, F., & Cueto, E. (2023). Thermodynamics-informed neural networks for physically realistic mixed reality. *Computer Methods in Applied Mechanics and Engineering*, *407*, 115912.

Damping effects of violent sloshing in airplane wings

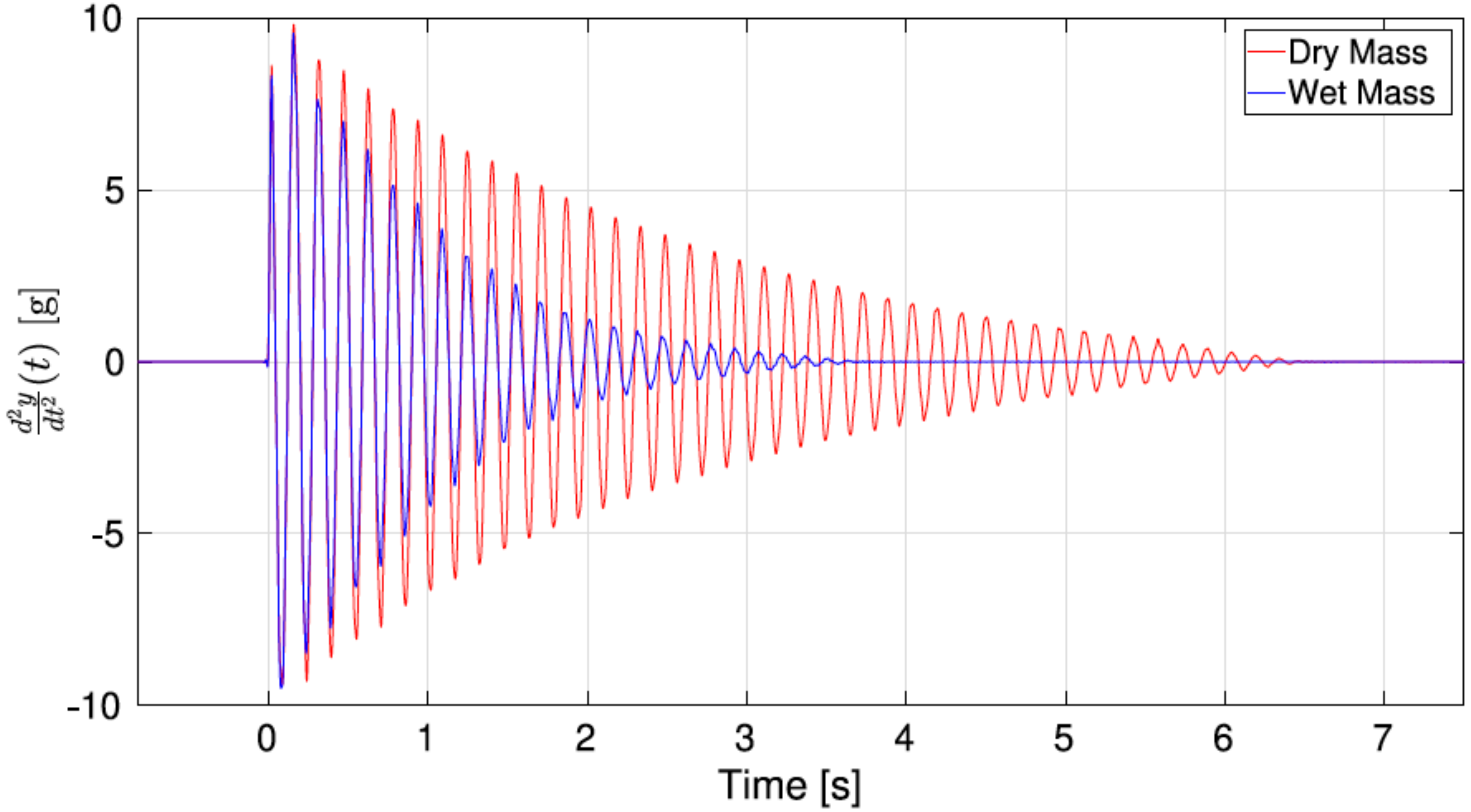
Experimental study of the liquid damping effects on a SDOF vertical sloshing tank.
J. Martinez-Carrascal, L.M. González-Gutierrez, Journal of Fluids and Structures, 2021





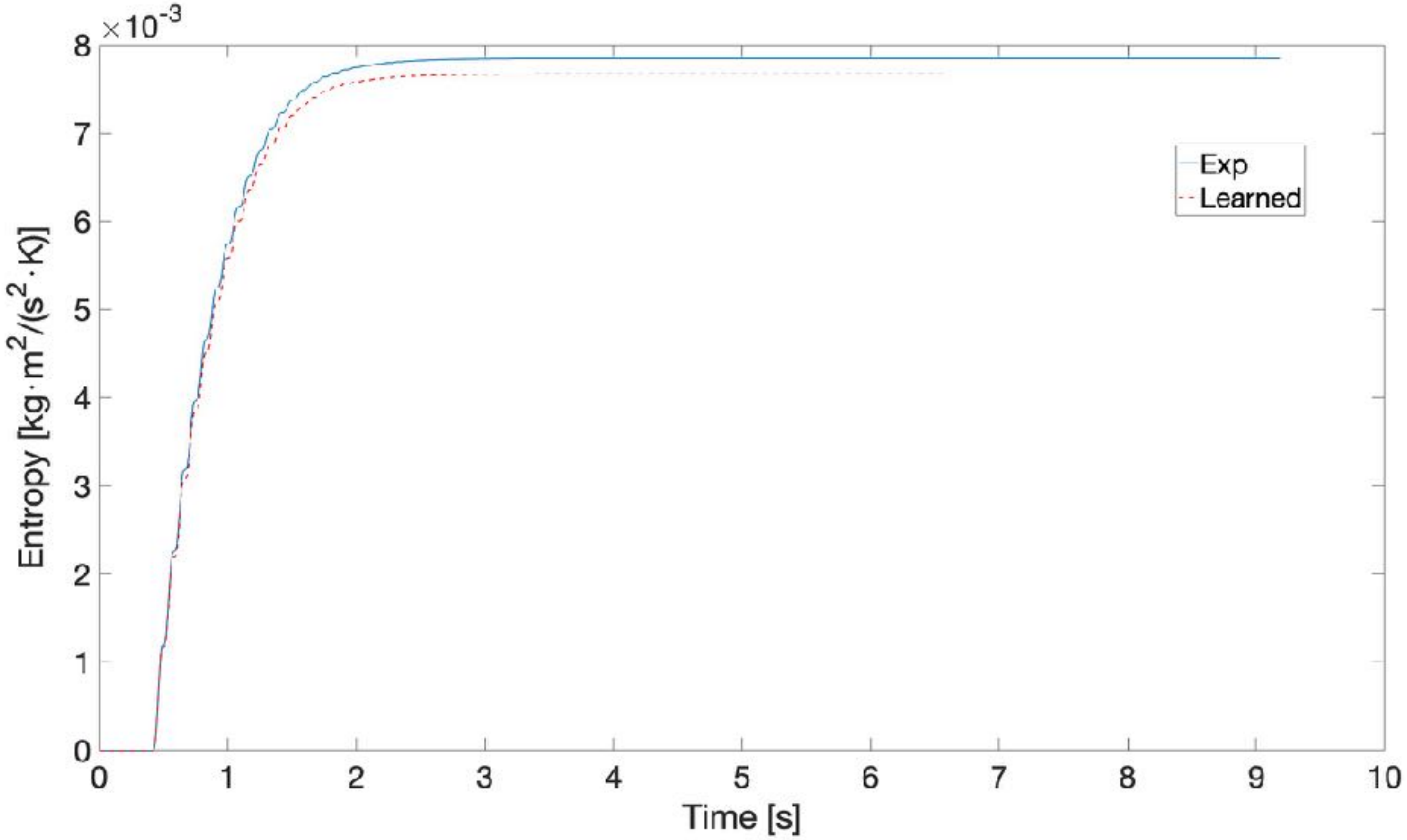
Learning strategy

- Characterize first the structural response of the tank
- Then learn the influence of different filling levels



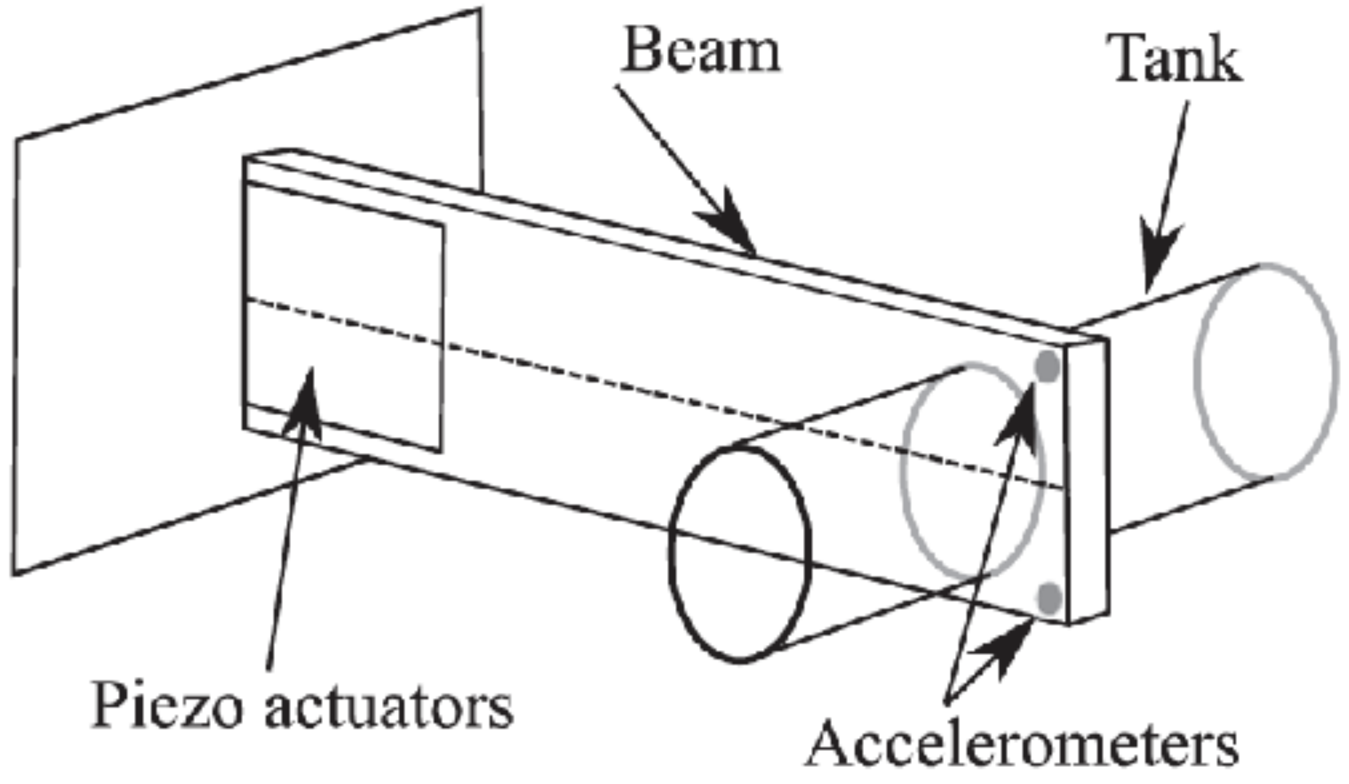
Experimental study of the liquid damping effects on a SDOF vertical sloshing tank.
J. Martinez-Carrascal, L.M. González-Gutierrez, Journal of Fluids and Structures, 2021

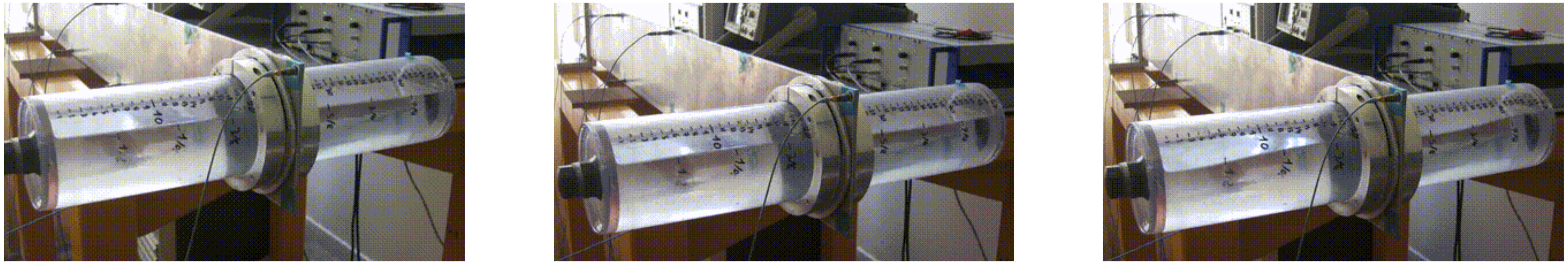
Variable damping due to sloshing



Fluid-structure interaction

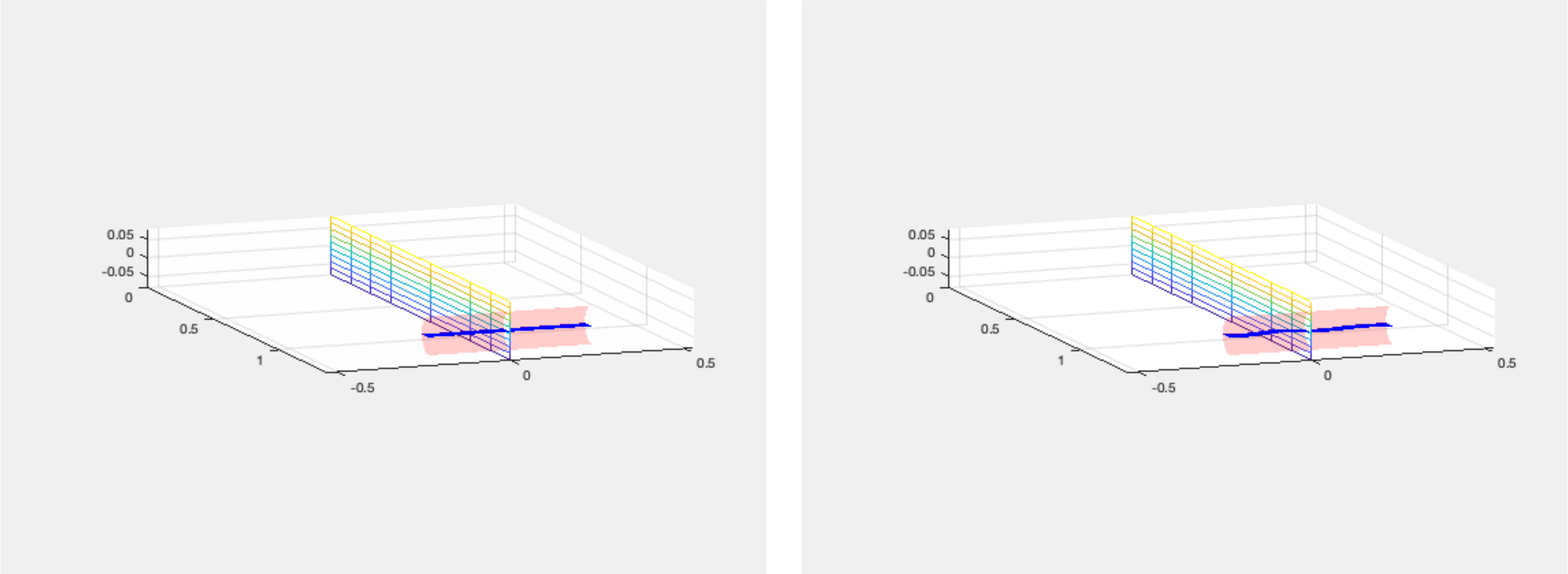
- Beam bending + torsion
- Rigid tank
- Sloshing fluid





A port-Hamiltonian model of liquid sloshing in moving containers and application to a fluid-structure system.
Flávio Luiz Cardoso-Ribeiro, Denis Matignon, Valérie Pommier-Budinger, Journal of Fluids and Structures, 2017.

Fluid-structure interaction

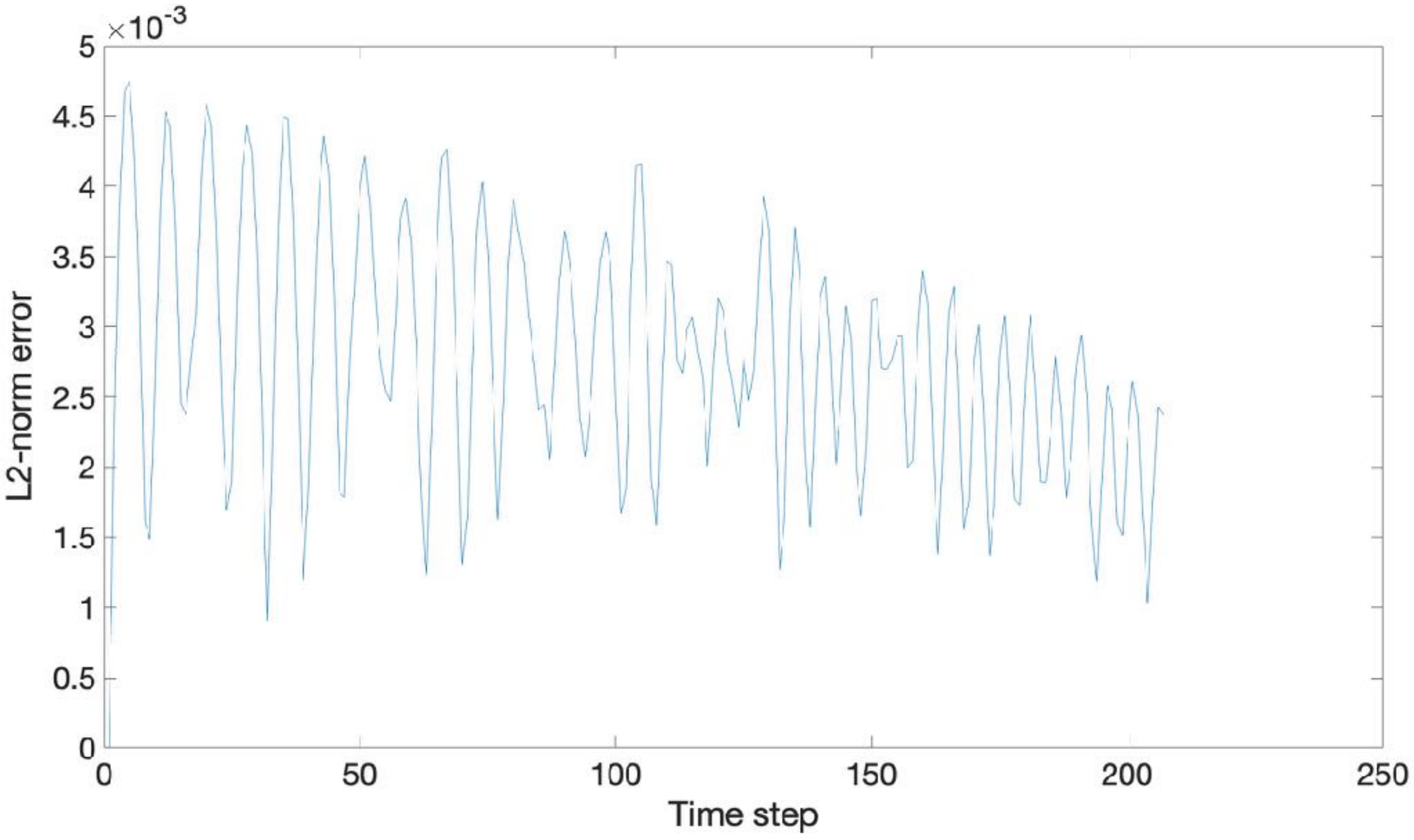


Reference

Learned

Fluid-structure interaction

- L2-norm error in the water free surface

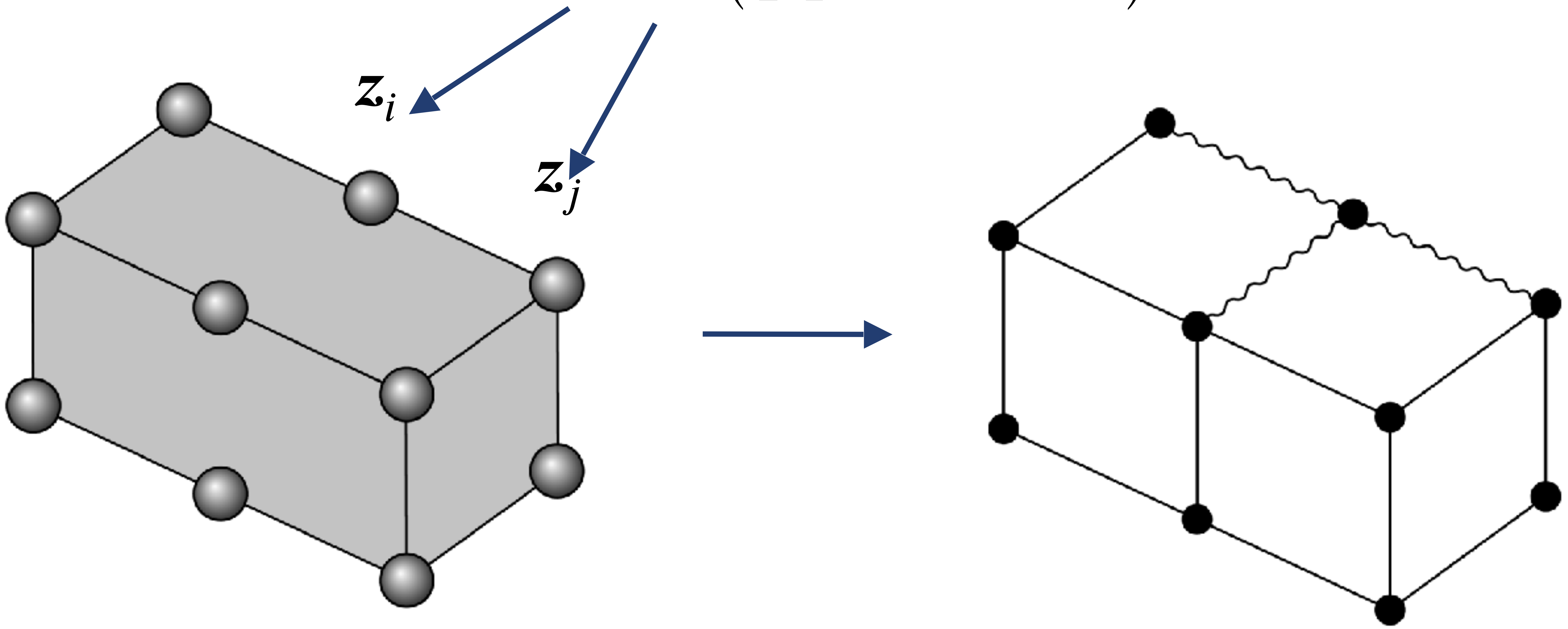


Contents

Geometric bias

- Graph construction

$$\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{p}, \boldsymbol{\sigma}, P, T, \ldots)$$

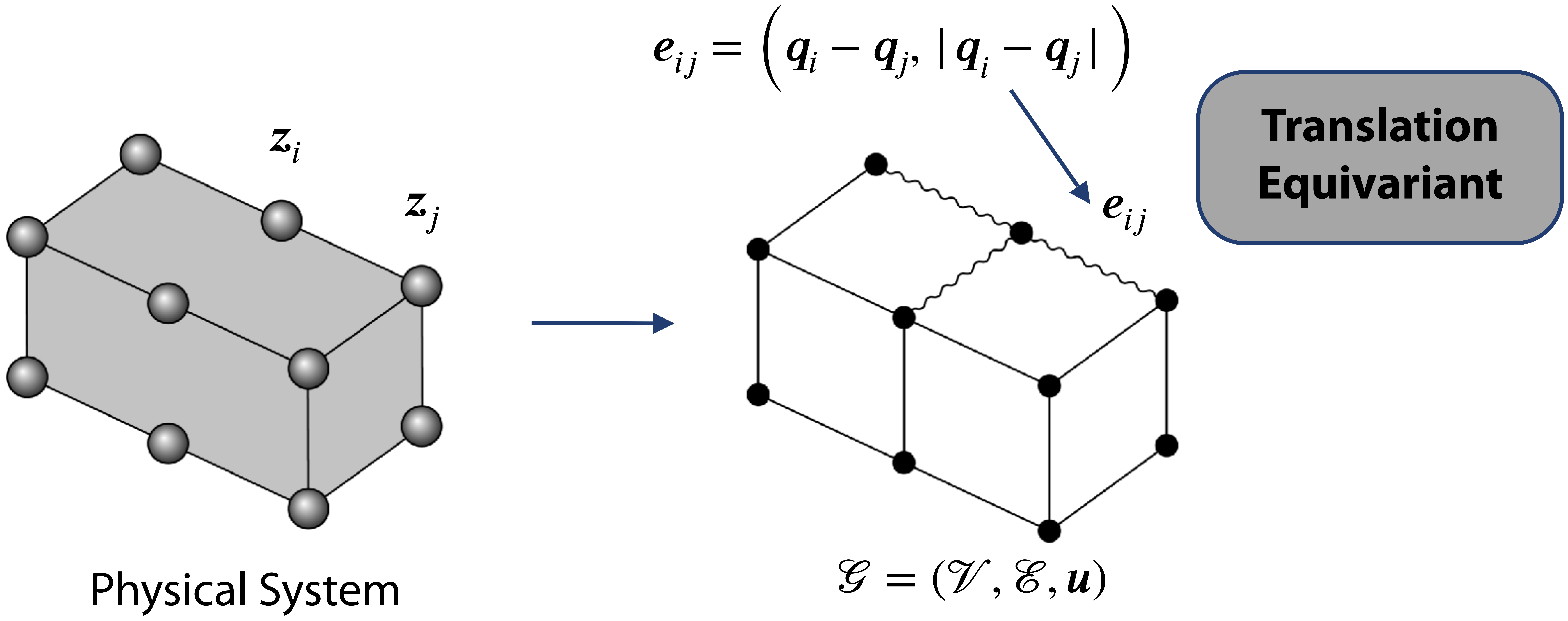


Physical System

$$\mathcal{G} = (\mathcal{V}, \mathcal{E}, \boldsymbol{u})$$

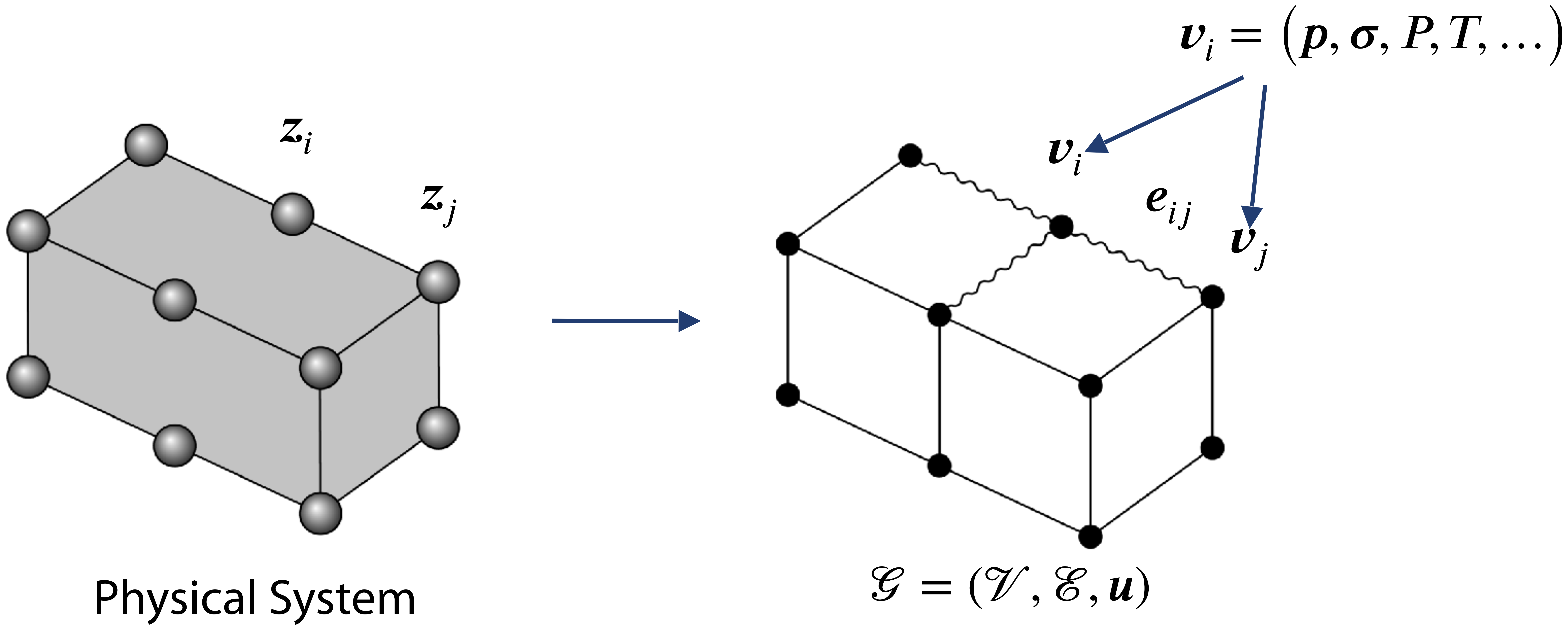
Geometric bias

- Graph construction



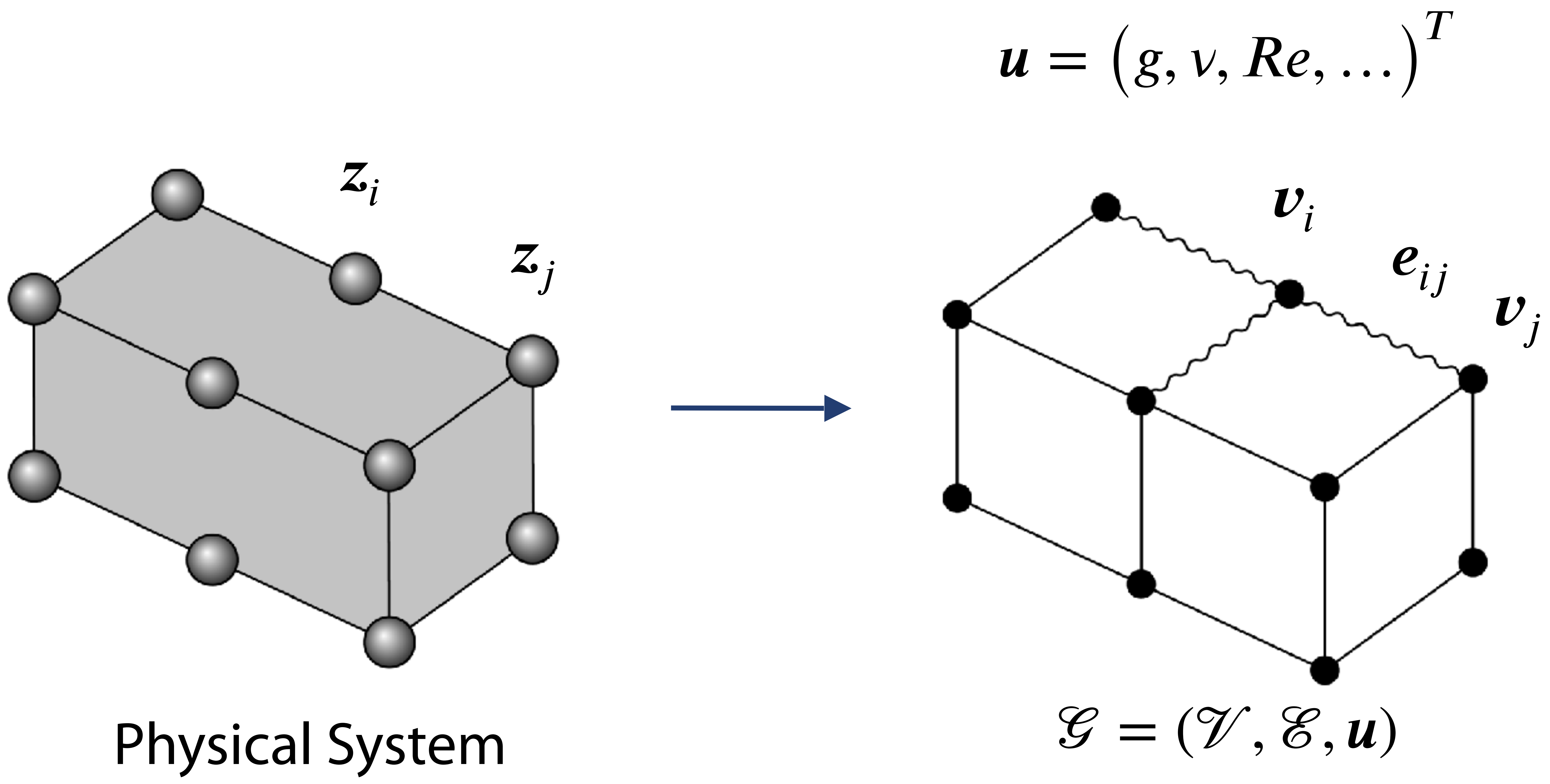
Geometric bias

- Graph construction



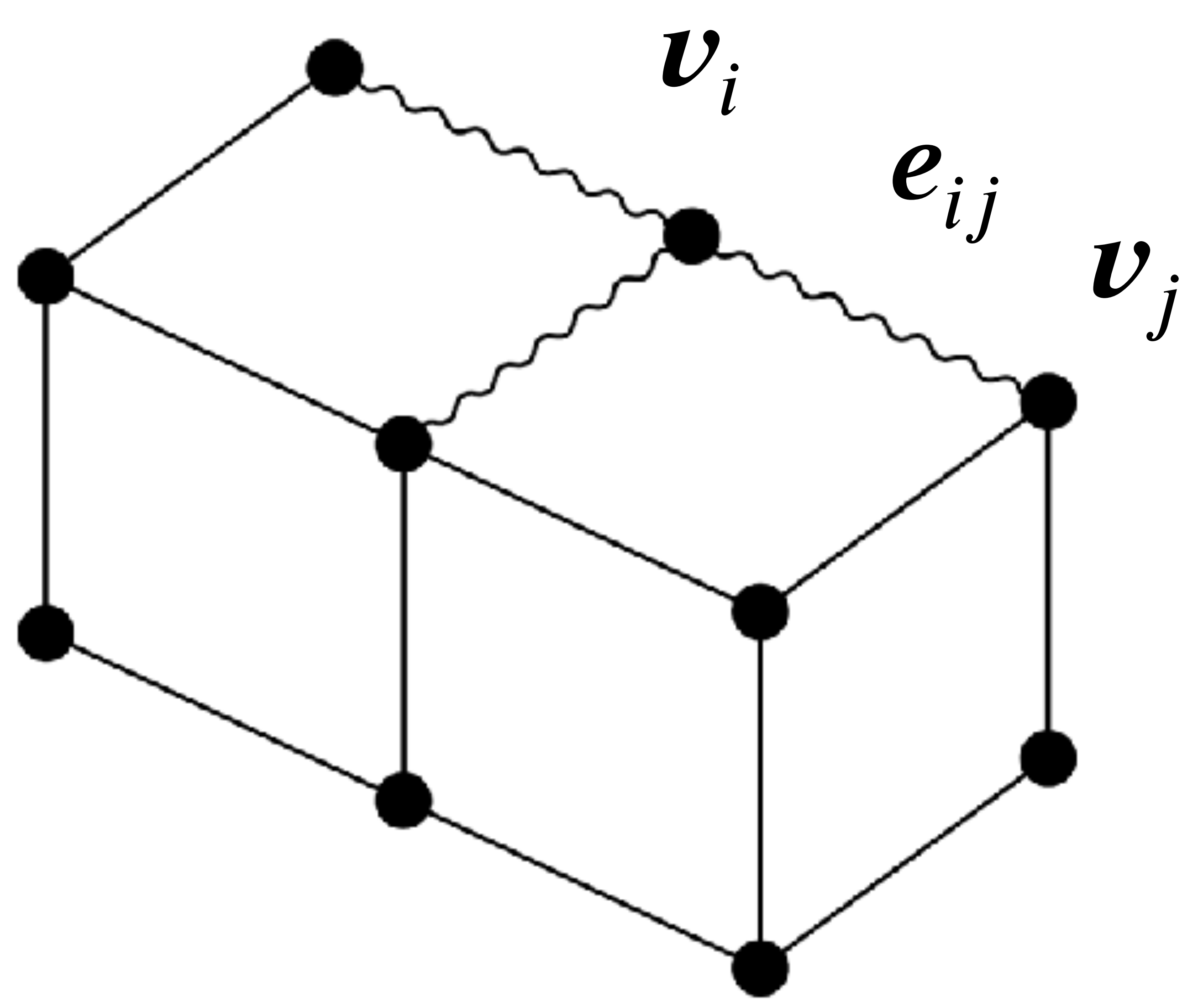
Geometric bias

- Graph construction



Geometric bias

- Encode – Process – Decode [Battaglia, 2018]

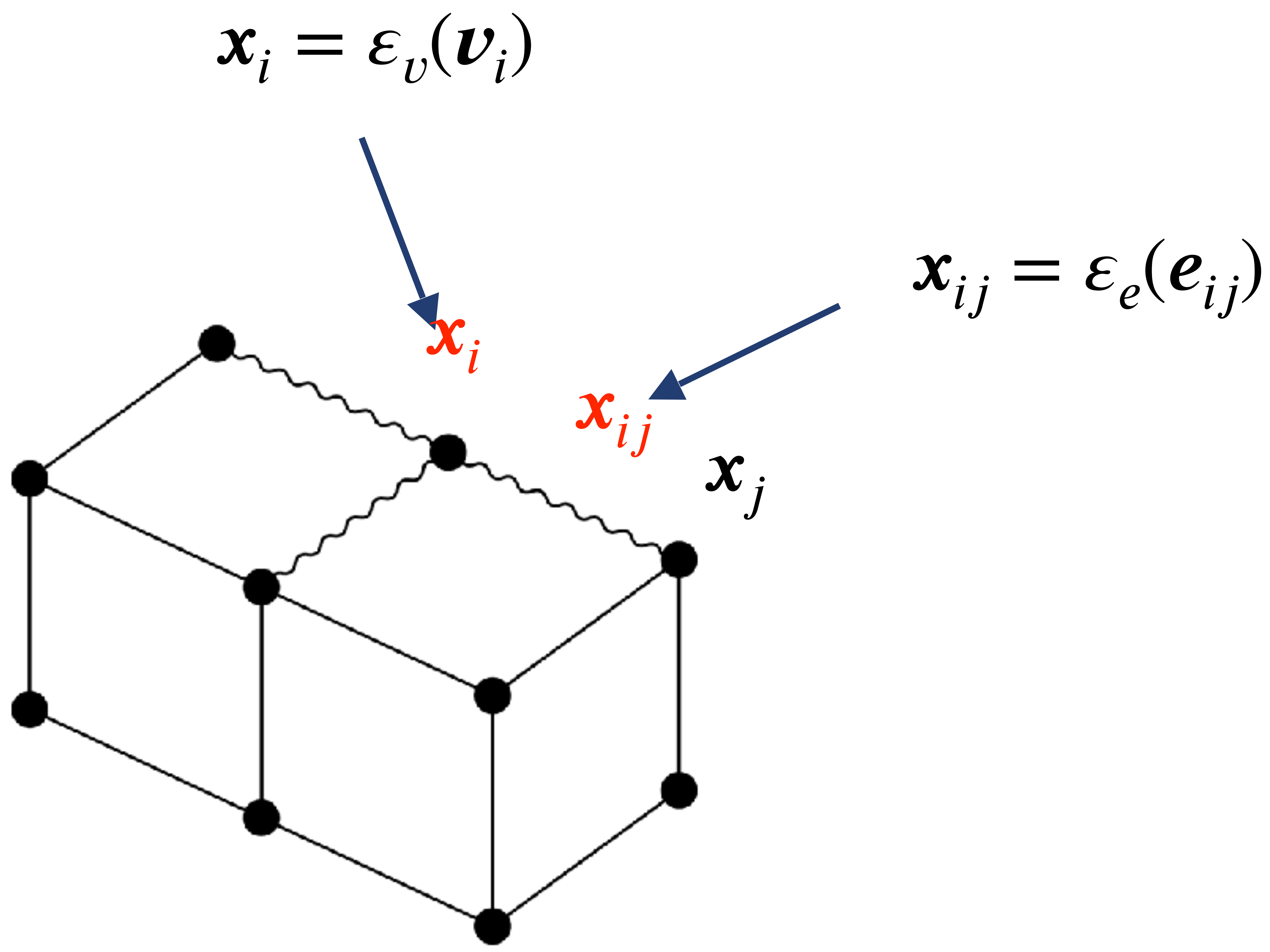


Geometric bias

- Encode – Process – Decode

[Battaglia, 2018]

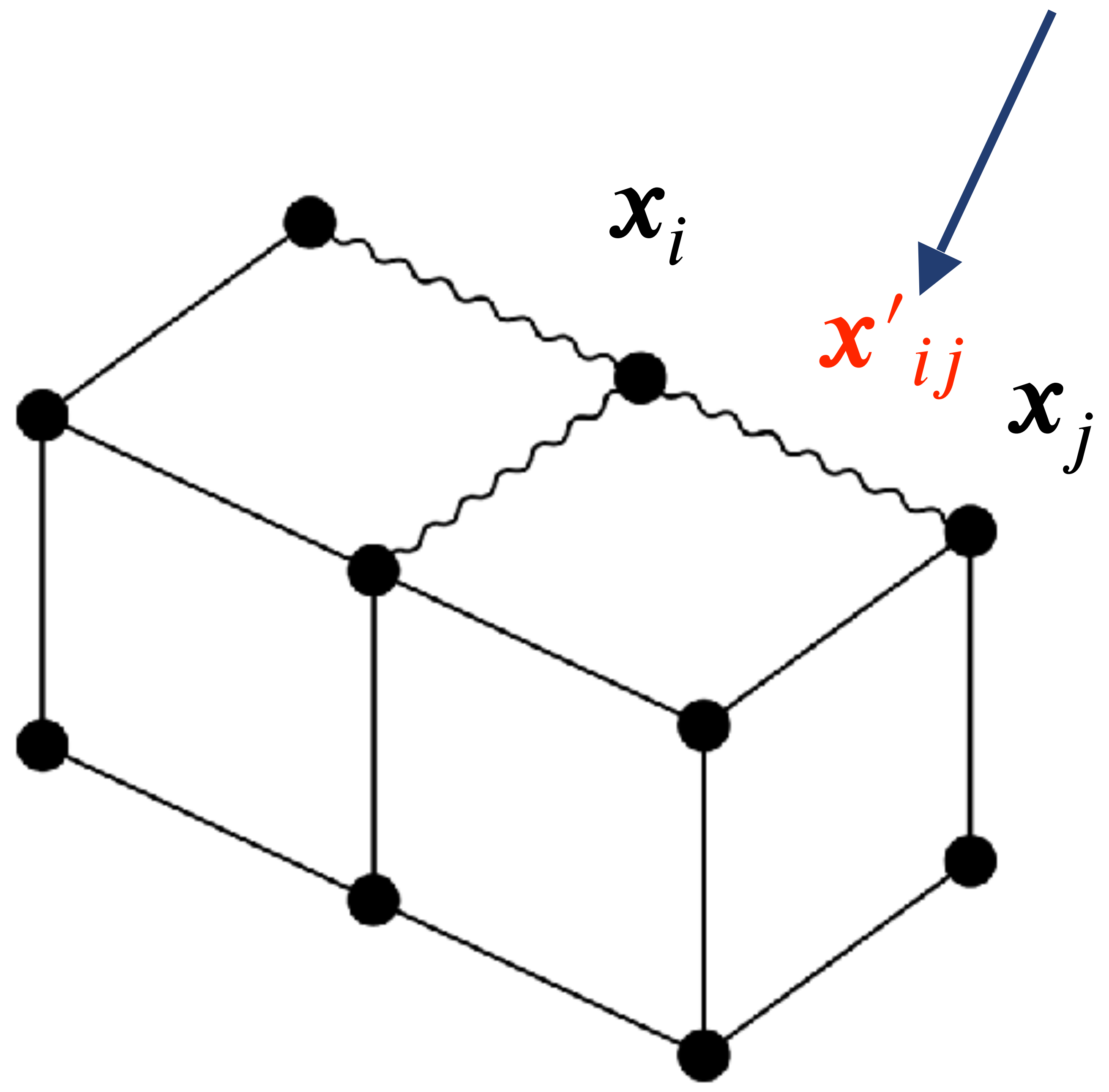
1. Encoder: $\varepsilon_v, \varepsilon_e$



Geometric bias

- Encode – Process – Decode [Battaglia, 2018]
  1. Encoder: $\varepsilon_v, \varepsilon_e$
  2. Update Edges: π_e

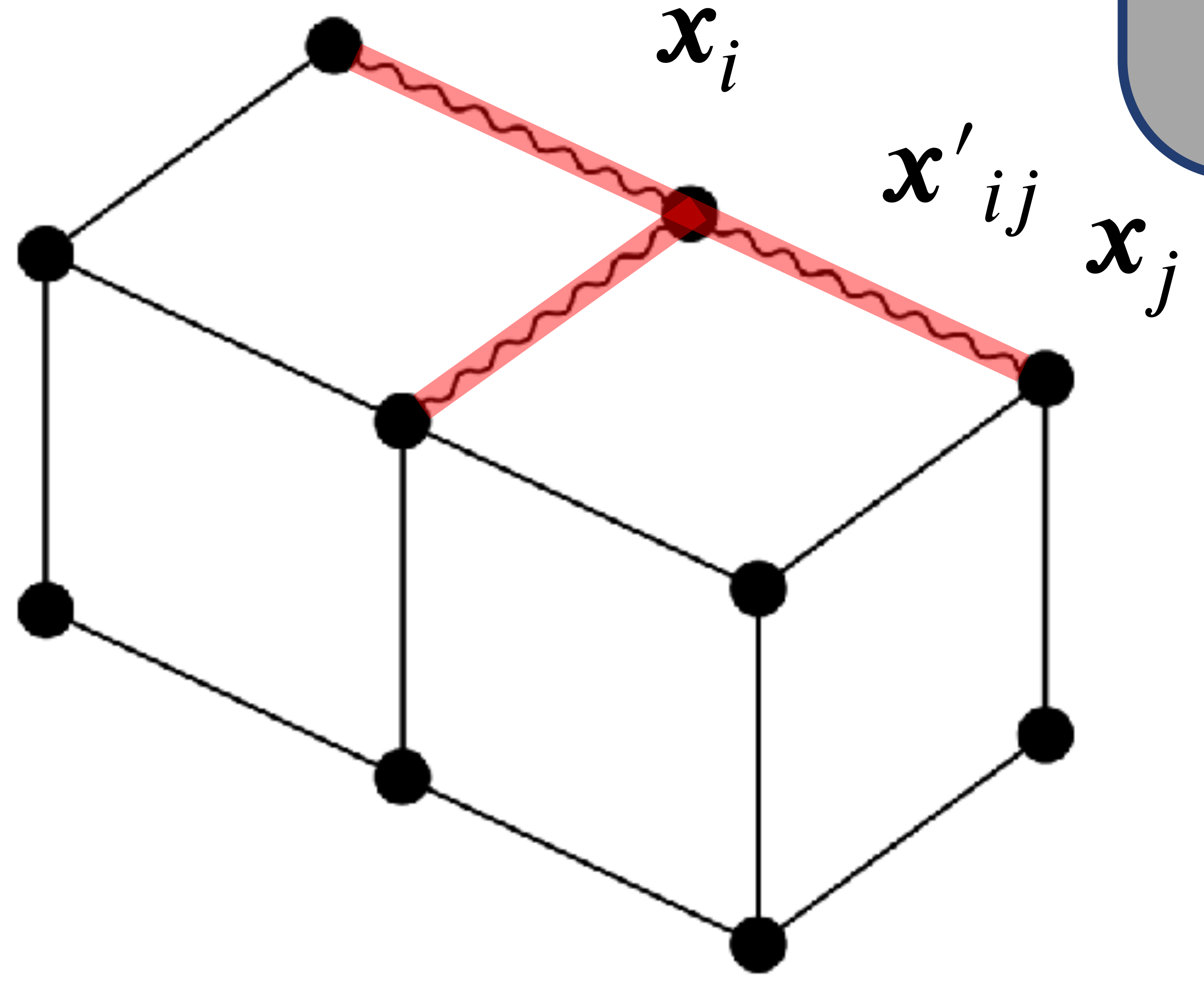
$$\boldsymbol{x}'_{ij} = \pi_e(\boldsymbol{x}_{ij}, \boldsymbol{x}_i, \boldsymbol{x}_j, \boldsymbol{u})$$



Geometric bias

- Encode – Process – Decode [Battaglia, 2018]
  1. Encoder: $\varepsilon_v, \varepsilon_e$
  2. Update Edges: π_e
  3. Message Passing

$$\boldsymbol{m}_i = \sum_{j \in \mathcal{N}_i} \boldsymbol{x}'_{ij}$$



Permutation Equivariant

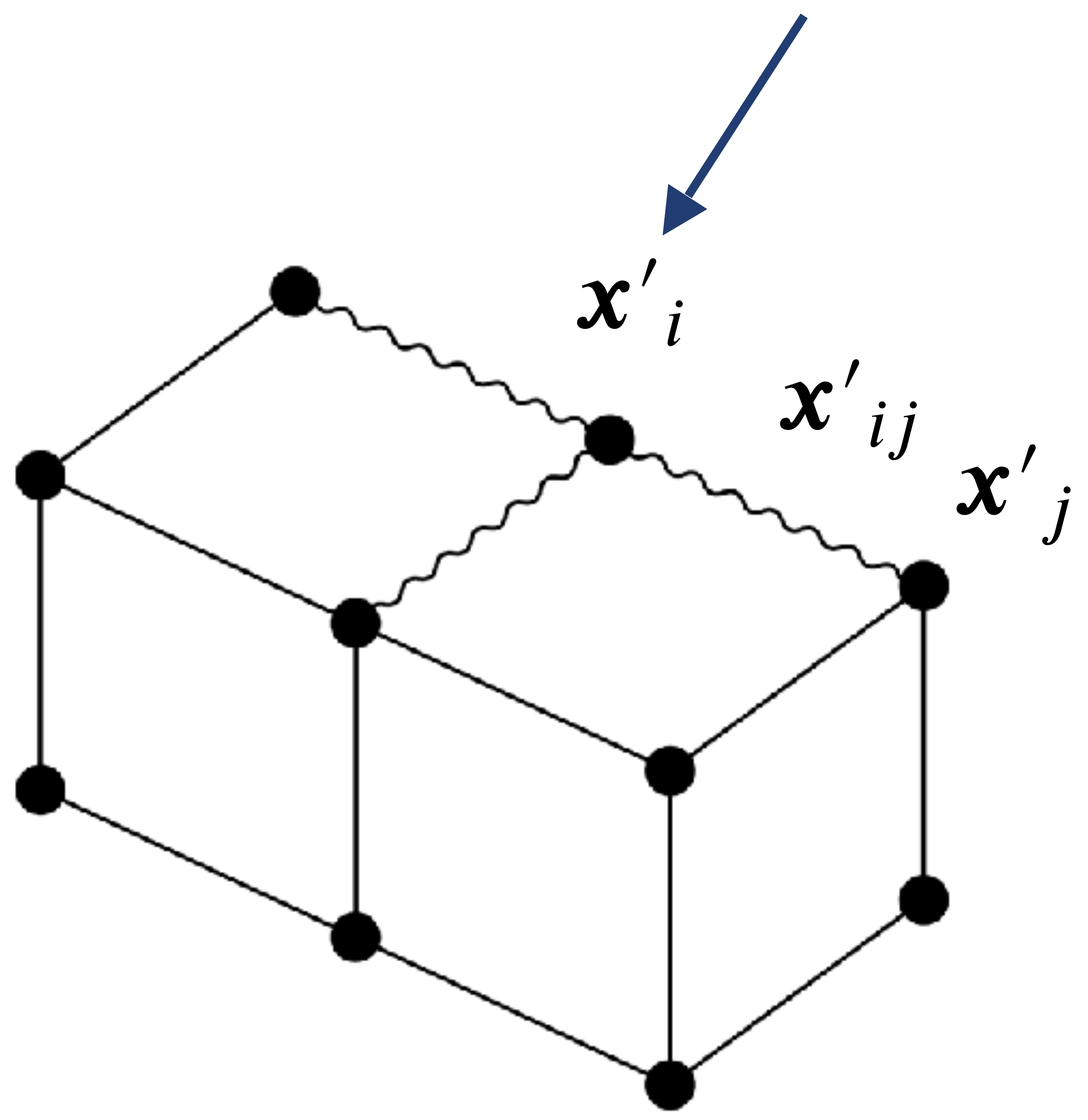
Geometric bias

- Encode – Process – Decode

[Battaglia, 2018]

1. Encoder: $\varepsilon_v, \varepsilon_e$
2. Update Edges: π_e
3. Message Passing
4. Update Vertices: π_v

$$\boldsymbol{x}'_i = \pi_v(\boldsymbol{m}_i, \boldsymbol{x}_i, \boldsymbol{u})$$

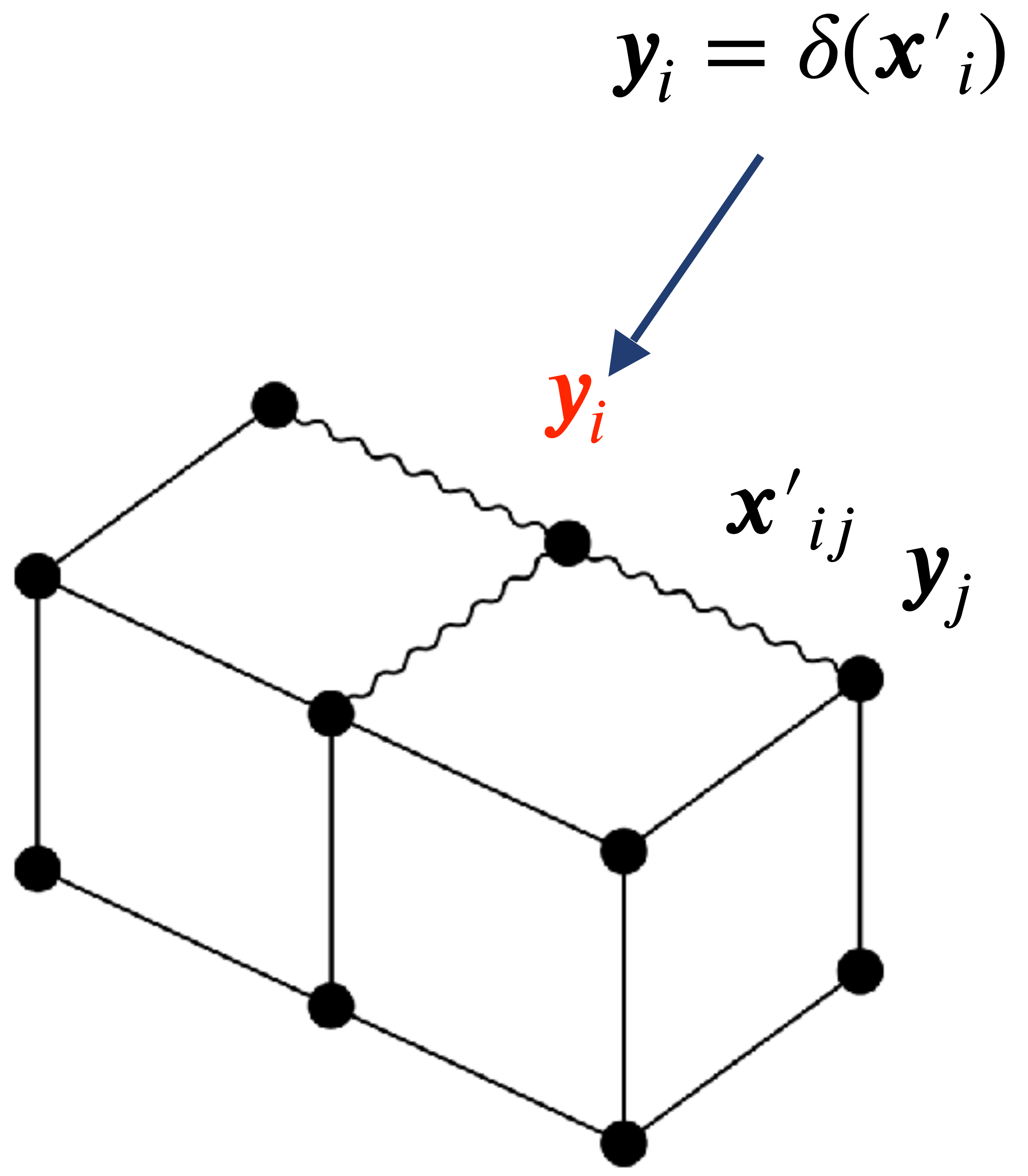


Geometric bias

- Encode – Process – Decode

[Battaglia, 2018]

1. Encoder: $\varepsilon_v, \varepsilon_e$
2. Update Edges: π_e
3. Message Passing
4. Update Vertices: π_v
5. Decoder: δ



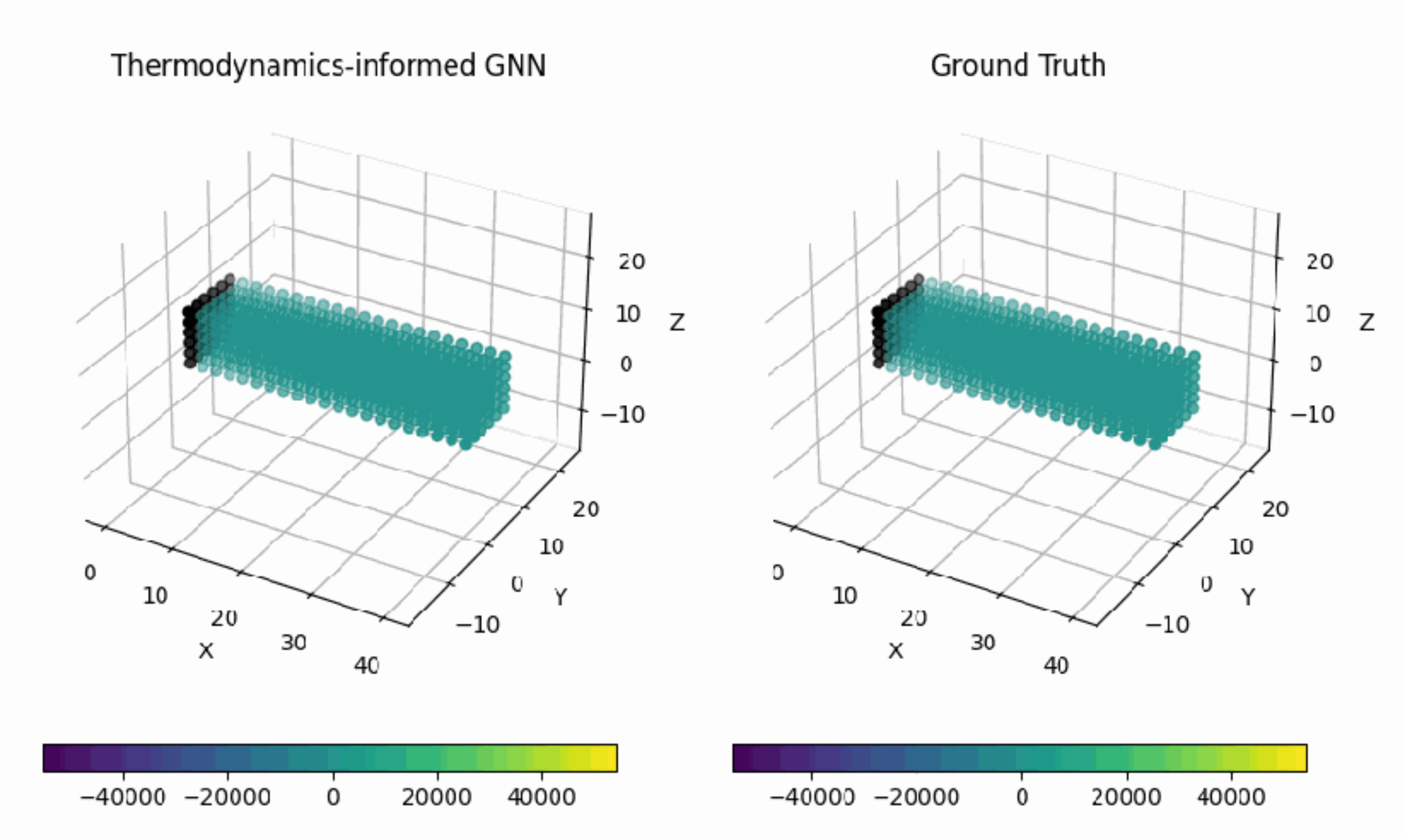
Experiments

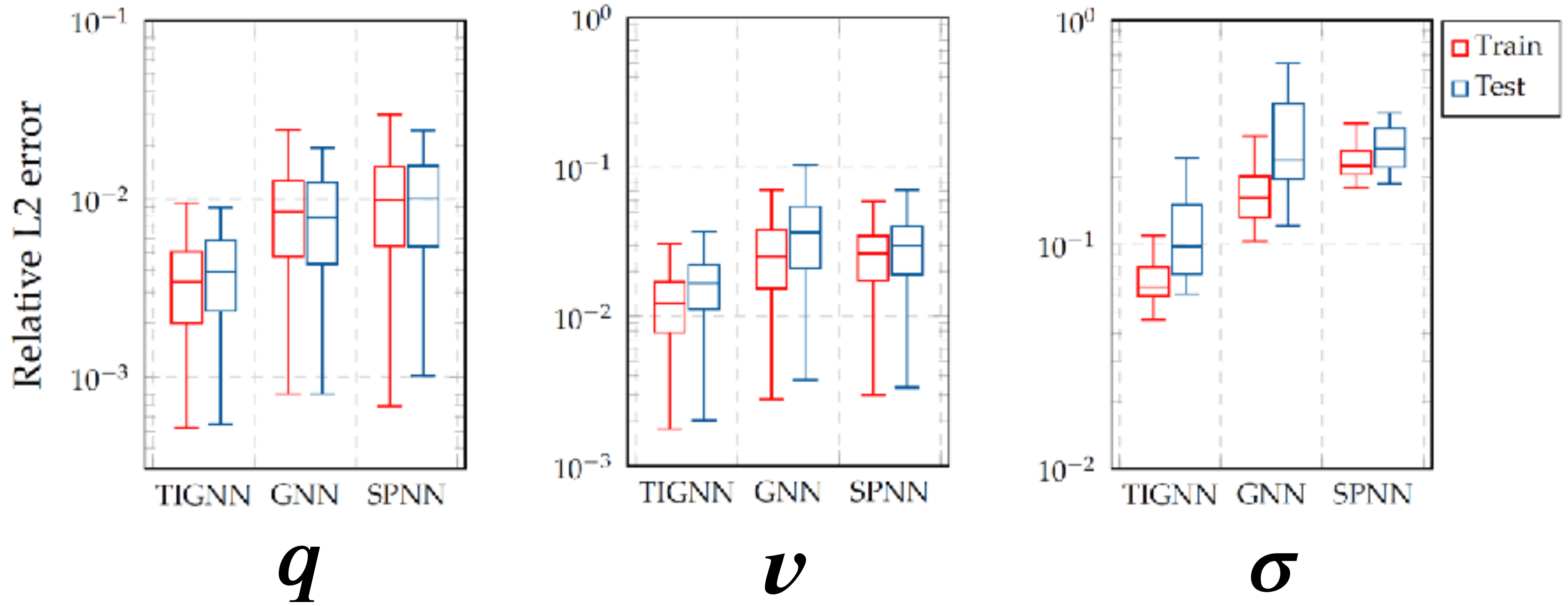
- Ablation study

Method	Physics	Geometry
SPNN [Hernández, 2021]	✓	✗
GNN [Pfaff, 2021]	✗	✓
TIGNN [Hernández, 2022]	✓	✓

Experiments

- Bending viscoelastic beam
  - State Space: $\mathcal{S} = \{\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{v}, \boldsymbol{\sigma})\}$
  - Dataset: 52 load positions





Experiments

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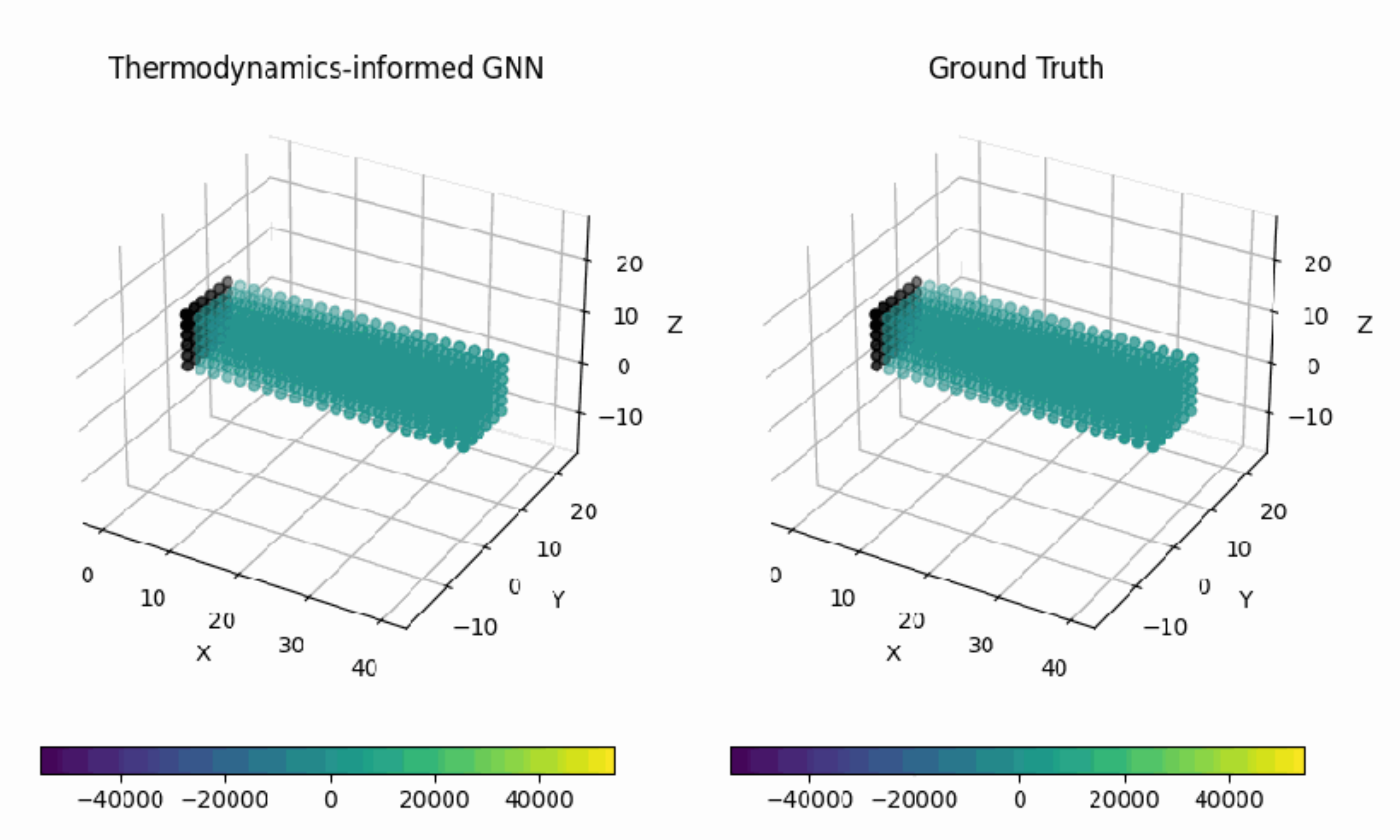
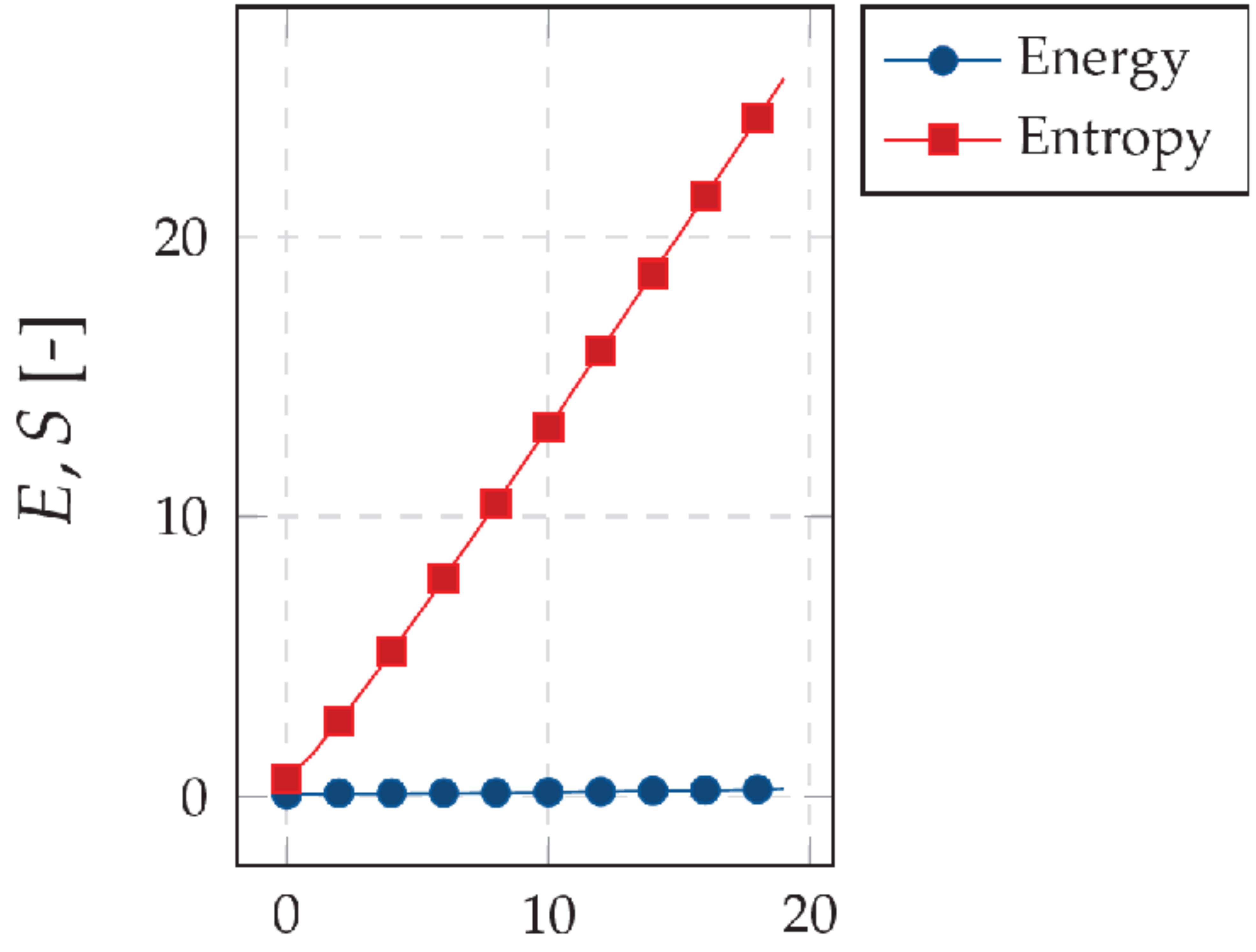
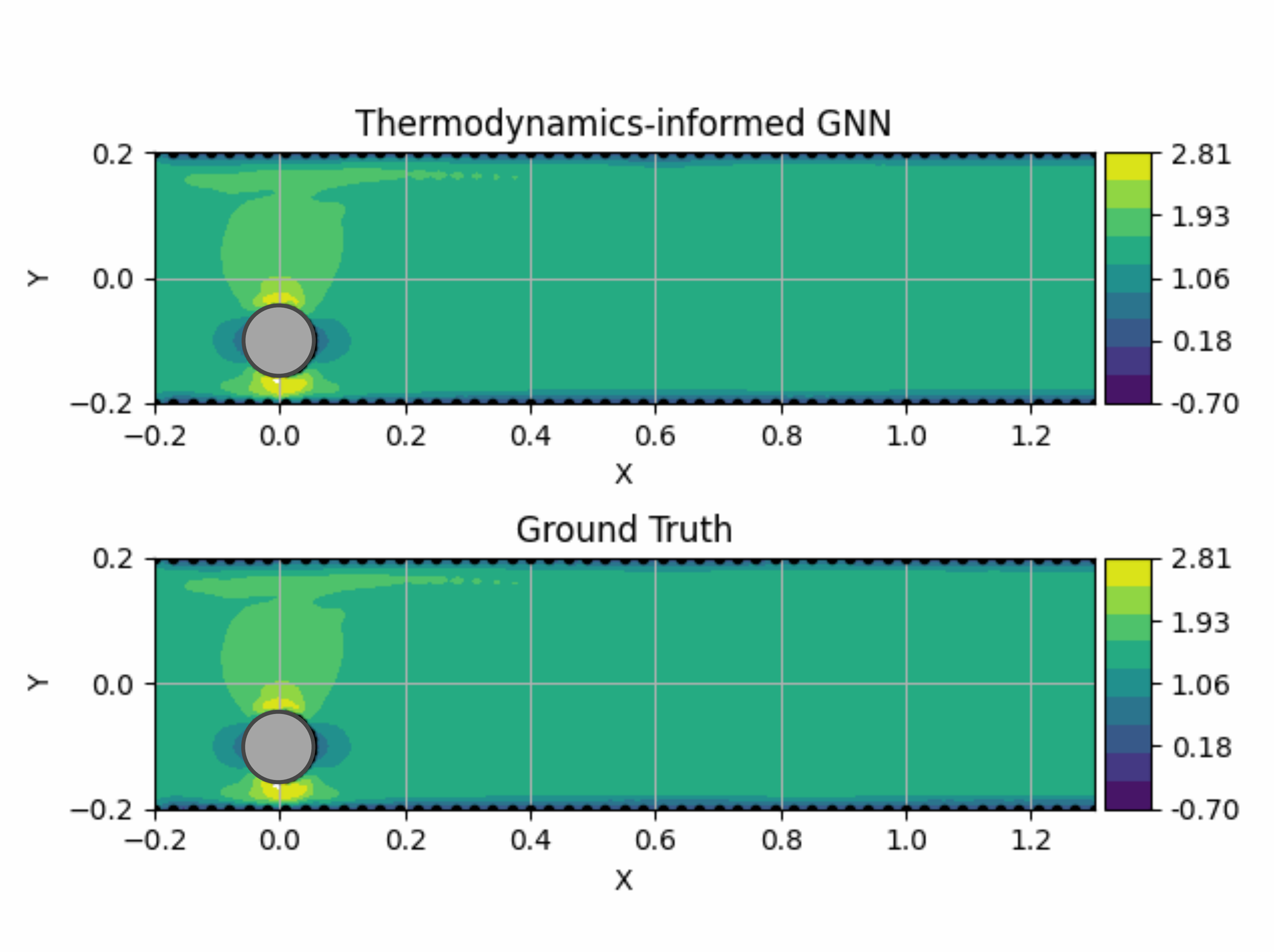
  - State Space: $\mathcal{S} = \{\boldsymbol{z} = (\boldsymbol{q}, \boldsymbol{v}, \boldsymbol{\sigma})\}$
  - Dataset: 52 load positions

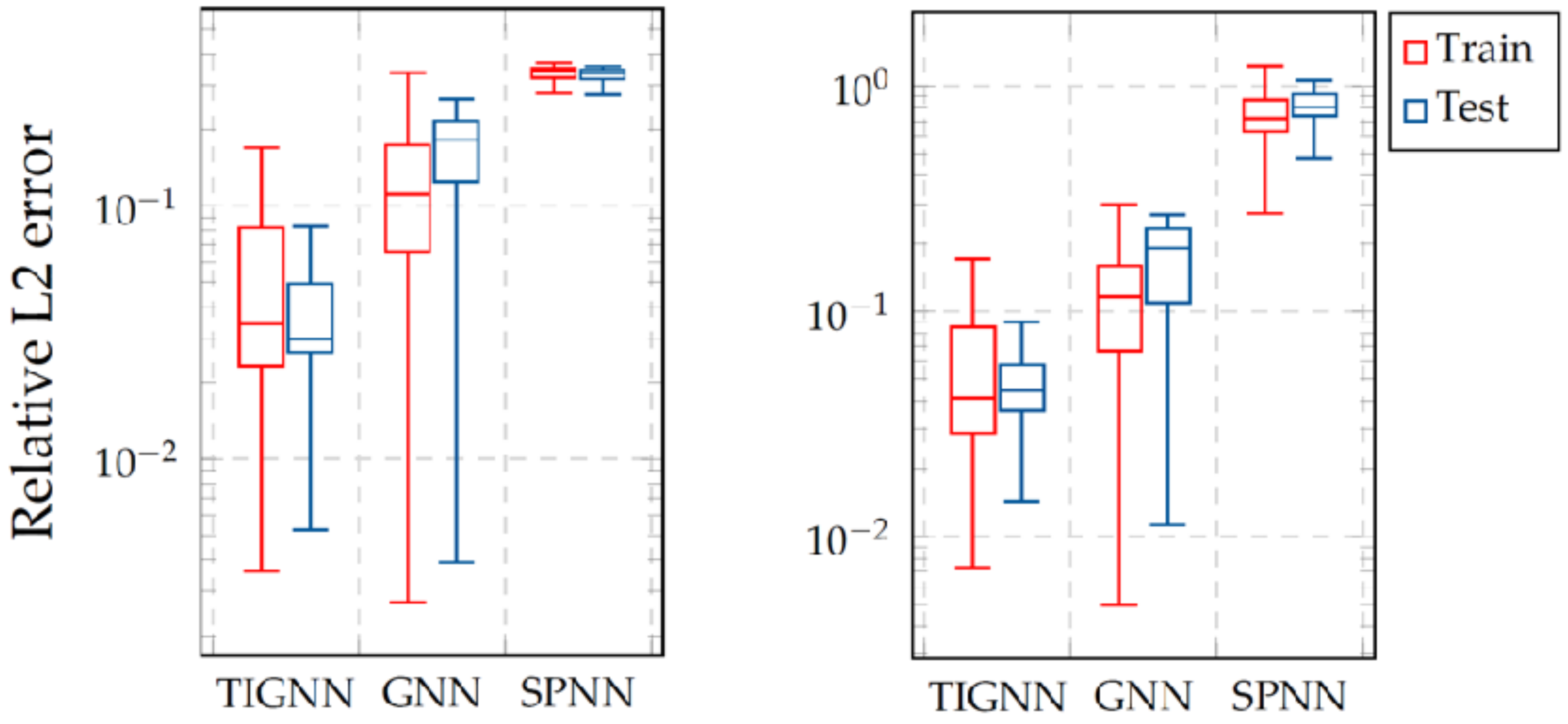




Experiments: previously unseen meshes

- Flow past a cylinder
  - State Space: $\mathcal{S} = \{\boldsymbol{z} = (\boldsymbol{v}, P)\}$
  - Dataset: 30 geometries + $\boldsymbol{v}$



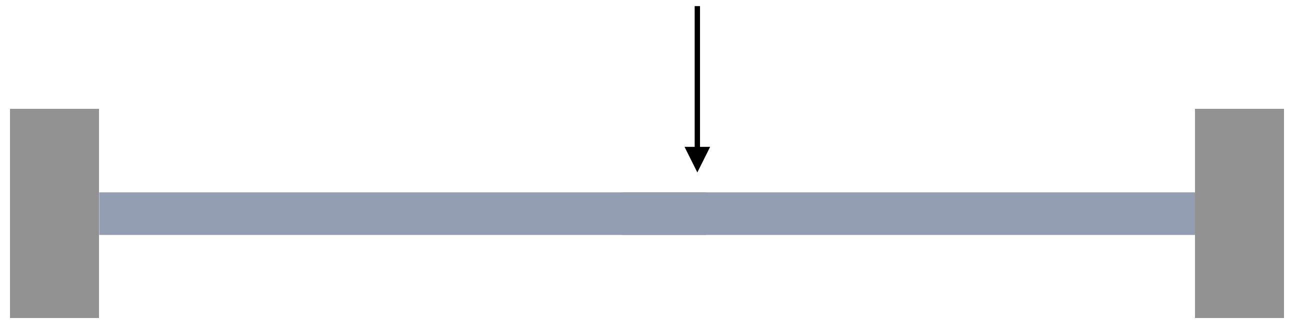


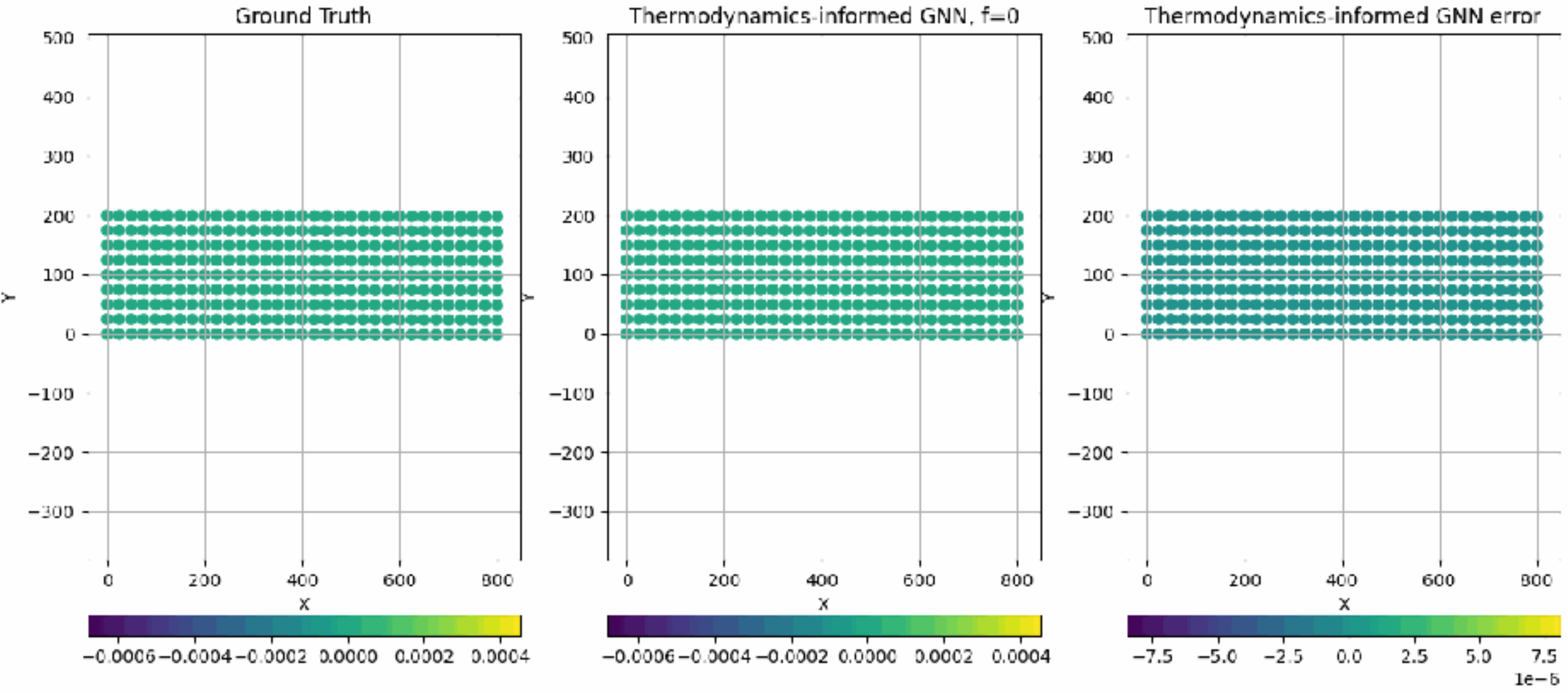
$\boldsymbol{v}$ $\qquad$ P

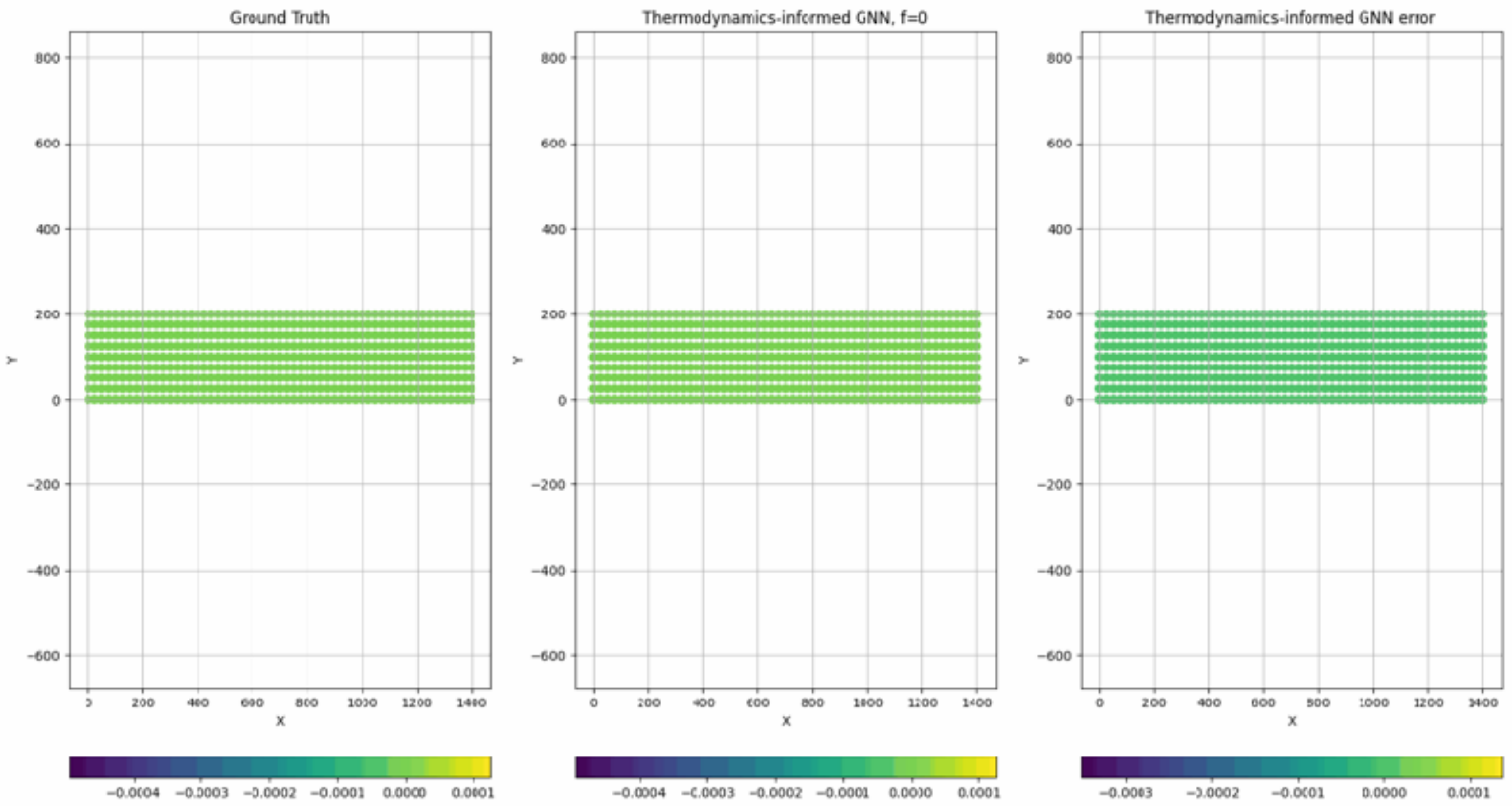
Are GNNs learning the physics?

Training:

Test:







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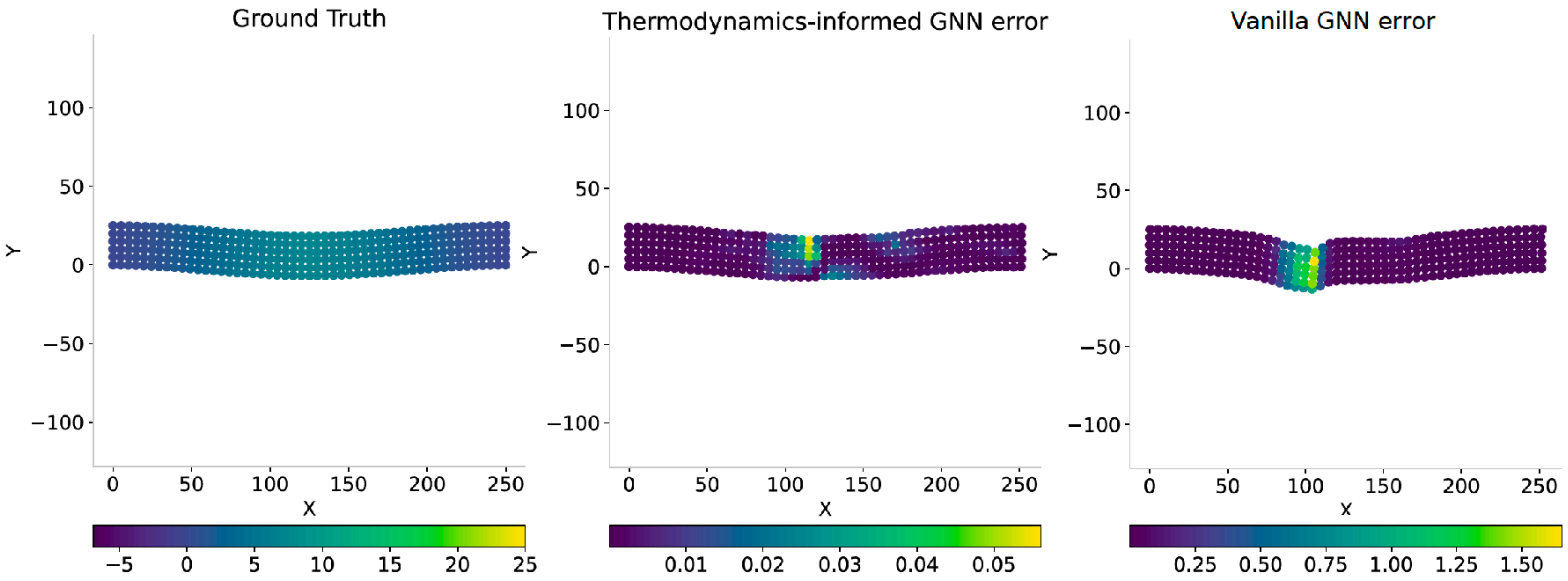
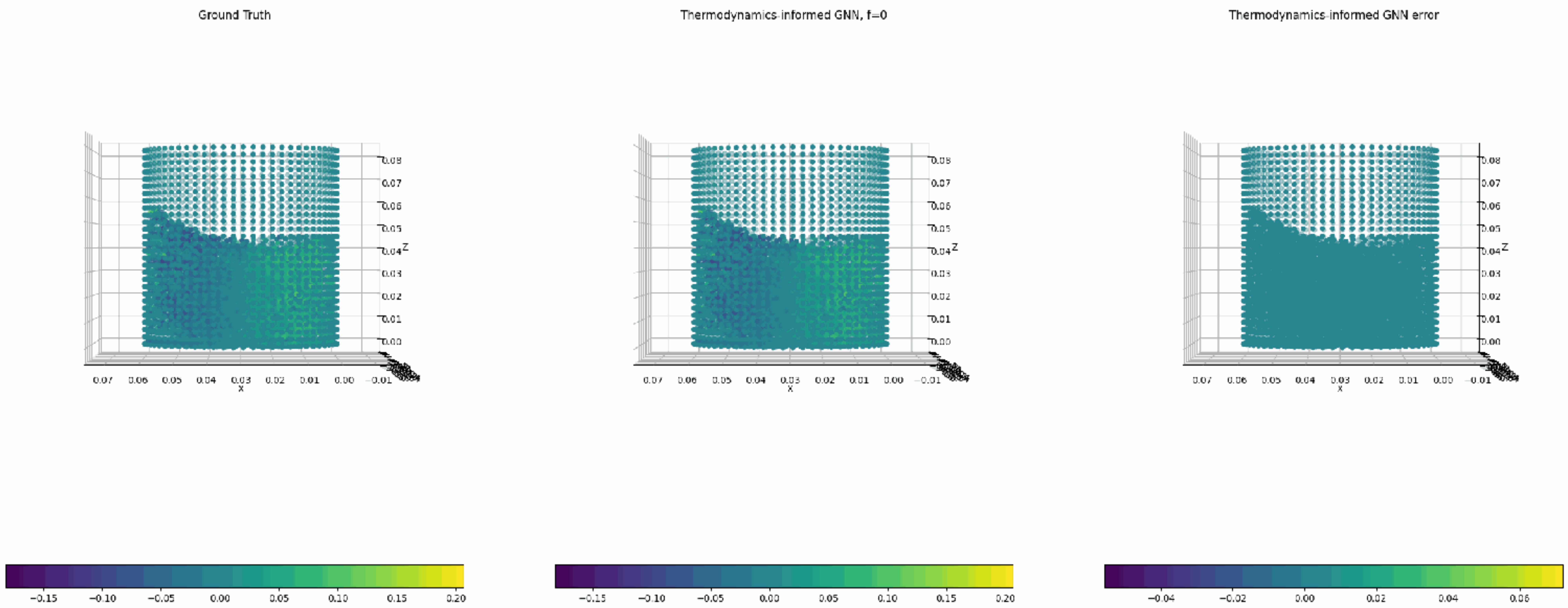
Are GNNs learning the physics?

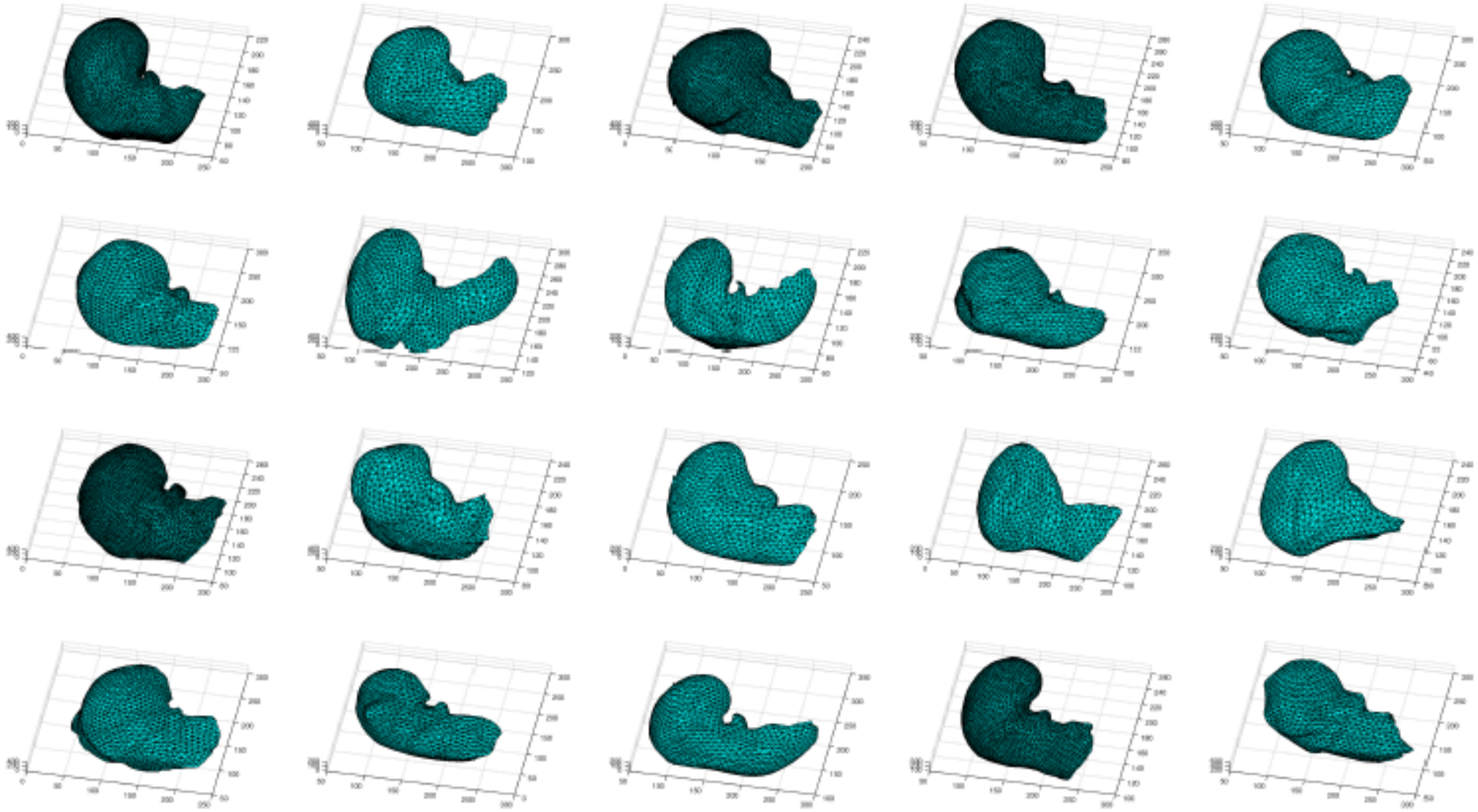


Previously unseen container geometry



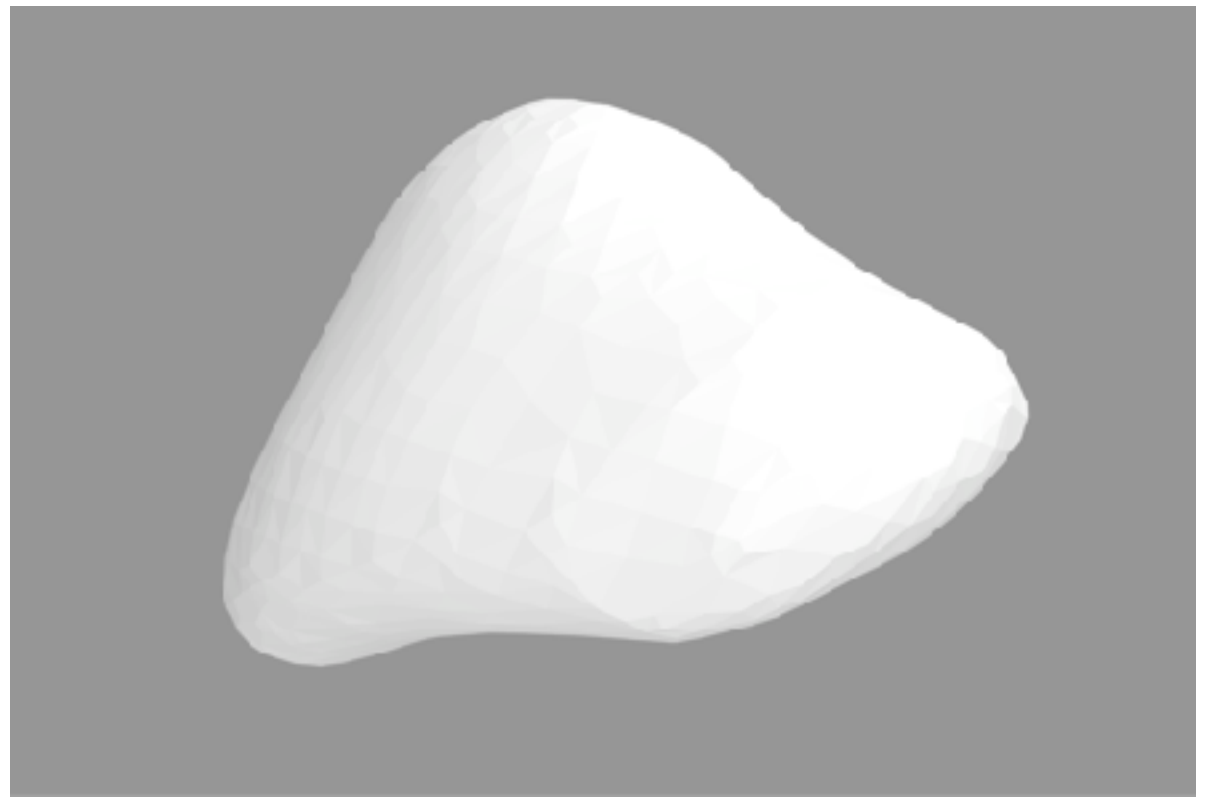
Digital human twins

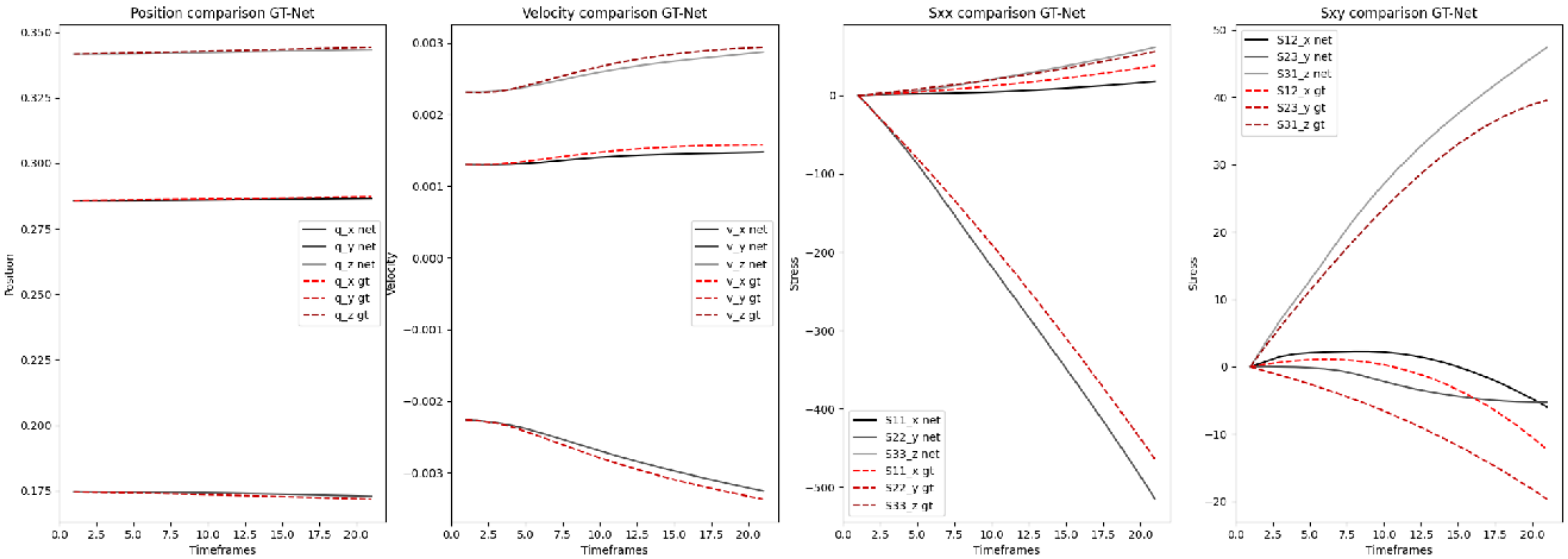
- Set of 20 actual liver anatomies provided by IRCAD, France



Ground truth vs. prediction

- Previously unseen anatomies





Conclusions

- Thermodynamics as inductive bias
- Robustness, accuracy
- Thermodynamics-informed GNNs as a promising choice
- Size matters!

+info, preprints, …

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Acknowledgements

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