

# Thermodynamics-informed Graph Neural Networks for anatomically accurate digital human twins

Lucas Tesán<sup>1</sup>, David González<sup>1</sup>, Francisco Chinesta<sup>2</sup>, Elías Cueto<sup>1</sup>

<sup>1</sup> Applied Mechanics and Bioengineering (AMB), ESI Group-UZ Chair of the National Strategy of AI. Instituto de Investigación en Ingeniería de Aragón (I3A), Universidad de Zaragoza, Mariano Esquillor s/n, 50018, Zaragoza, Spain.

<sup>2</sup> ESI Group Chair. PIMM Lab, Arts et Metiers Institute of Technology, Paris, France. CNRS@CREATE LTD, CNRS, Singapore

Real render of  
a liver 3D model:  
26x15x8 cm

## Problem:

We want to describe the dynamic system:

$$\dot{\mathbf{z}} = F(\mathbf{z}, t), \quad t \in I = (0, T], \quad \mathbf{z}(0) = \mathbf{z}_0,$$

$$\dot{\mathbf{z}}_{t+1} = \dot{\mathbf{z}}_t + \Delta t \dot{\mathbf{z}} = \dot{\mathbf{z}}_t + \boxed{F(t)} ?$$

## Keypoints:

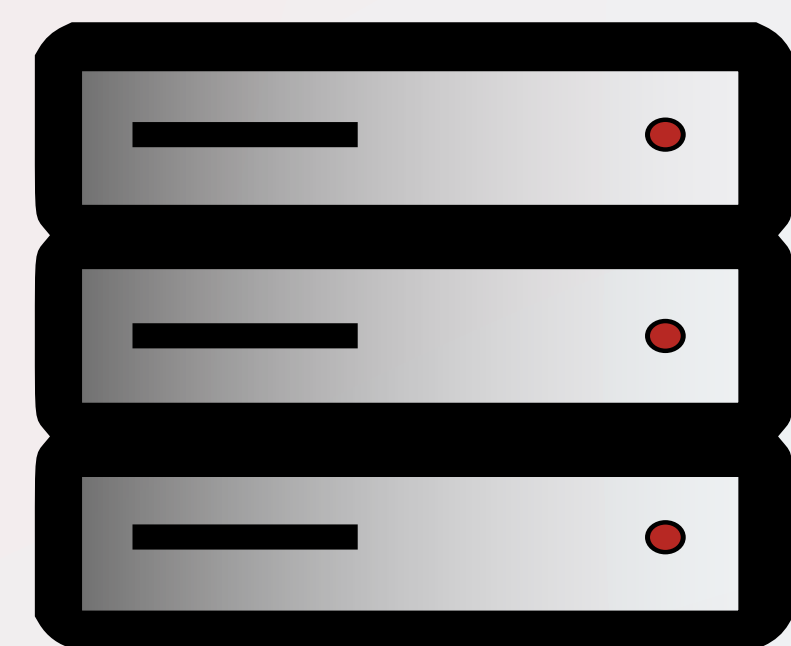
- **Real Time** Simulation
- **Mesh Independent** Solution
- Inductive Biases
- **Hybrid Artificial** Intelligence

## Methods and architecture:

**Mesh Preprocessing:**  
Low poly 3D model with  
volumetric meshing

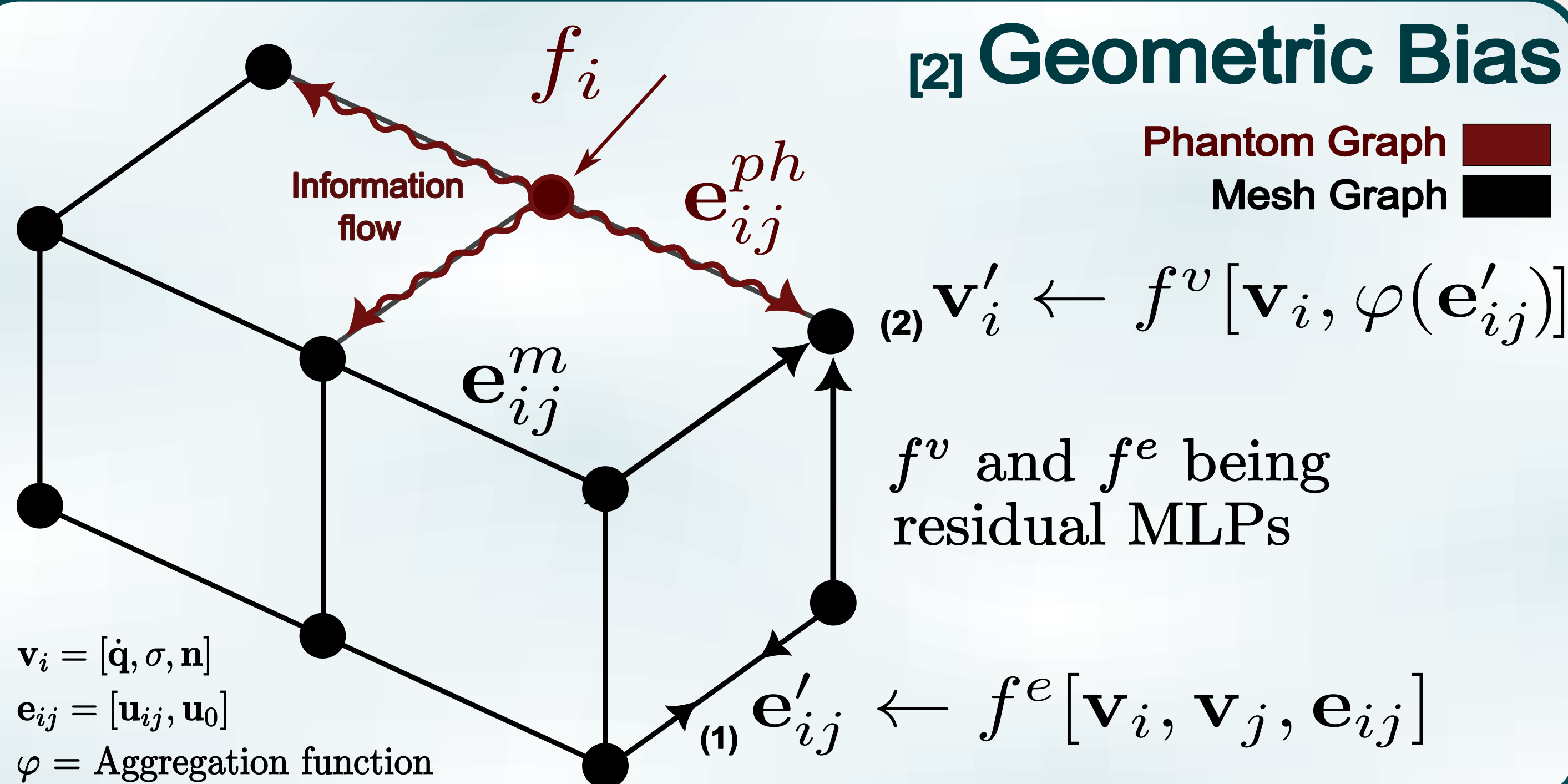
## Data Generation:

- Quasi-Static simulations
- Fixed nodes on visceral face
- Imposed displacement on 1 to 3 nodes
- Viscoelastic and Hyperelastic properties



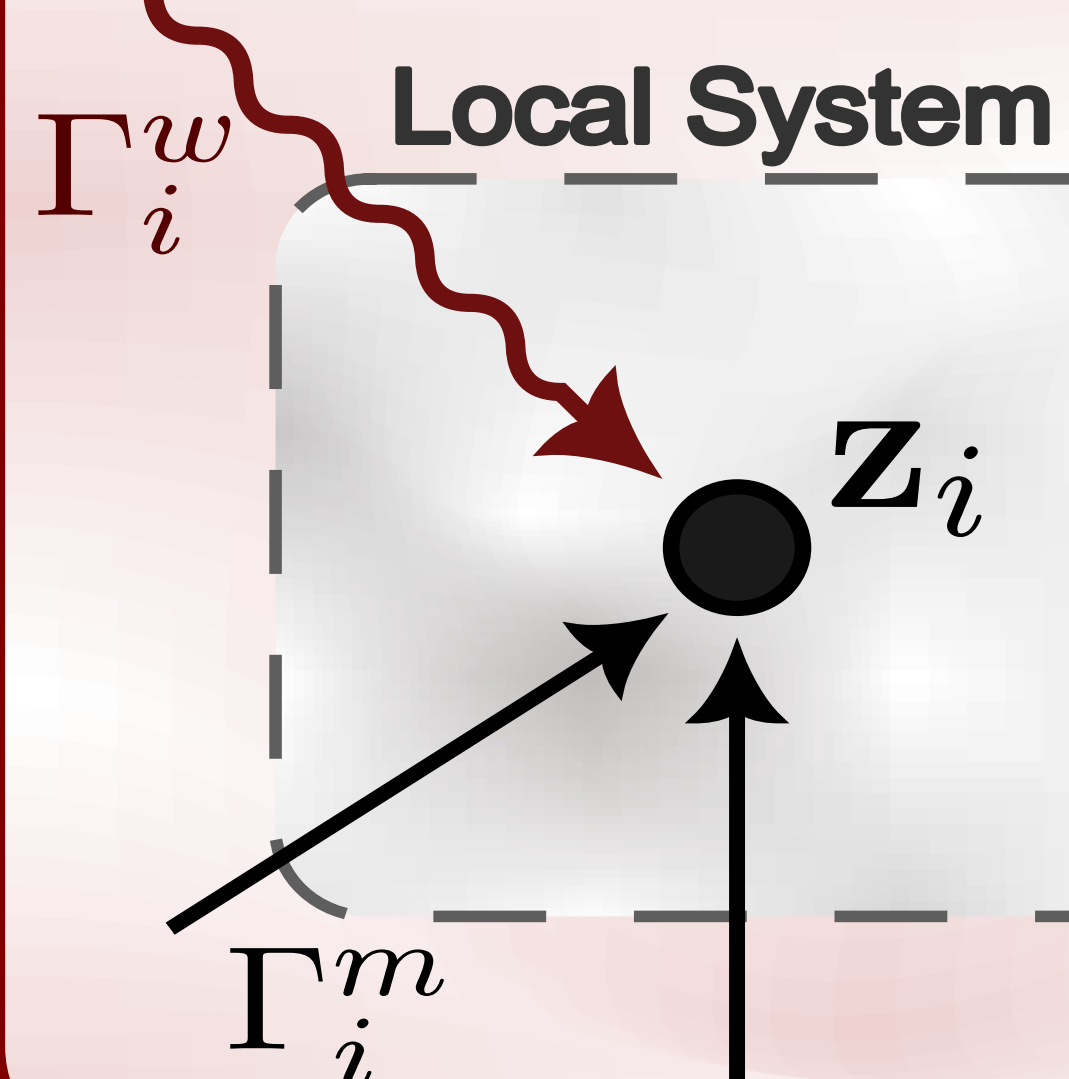
Database

## [2] Geometric Bias



## Boundary operator:

Energy and entropy exchange



## [1,3,4] Physic Bias

Fulfillment 1st and 2nd law of Thermodynamics

## Local GENERIC imposition

$$\dot{\mathbf{z}} = \mathbf{L} \frac{\partial E}{\partial \mathbf{z}} + \mathbf{M} \frac{\partial S}{\partial \mathbf{z}} - \mathbf{L}_\Gamma \frac{\partial E_\Gamma}{\partial \mathbf{z}} - \mathbf{M}_\Gamma \frac{\partial S_\Gamma}{\partial \mathbf{z}}$$

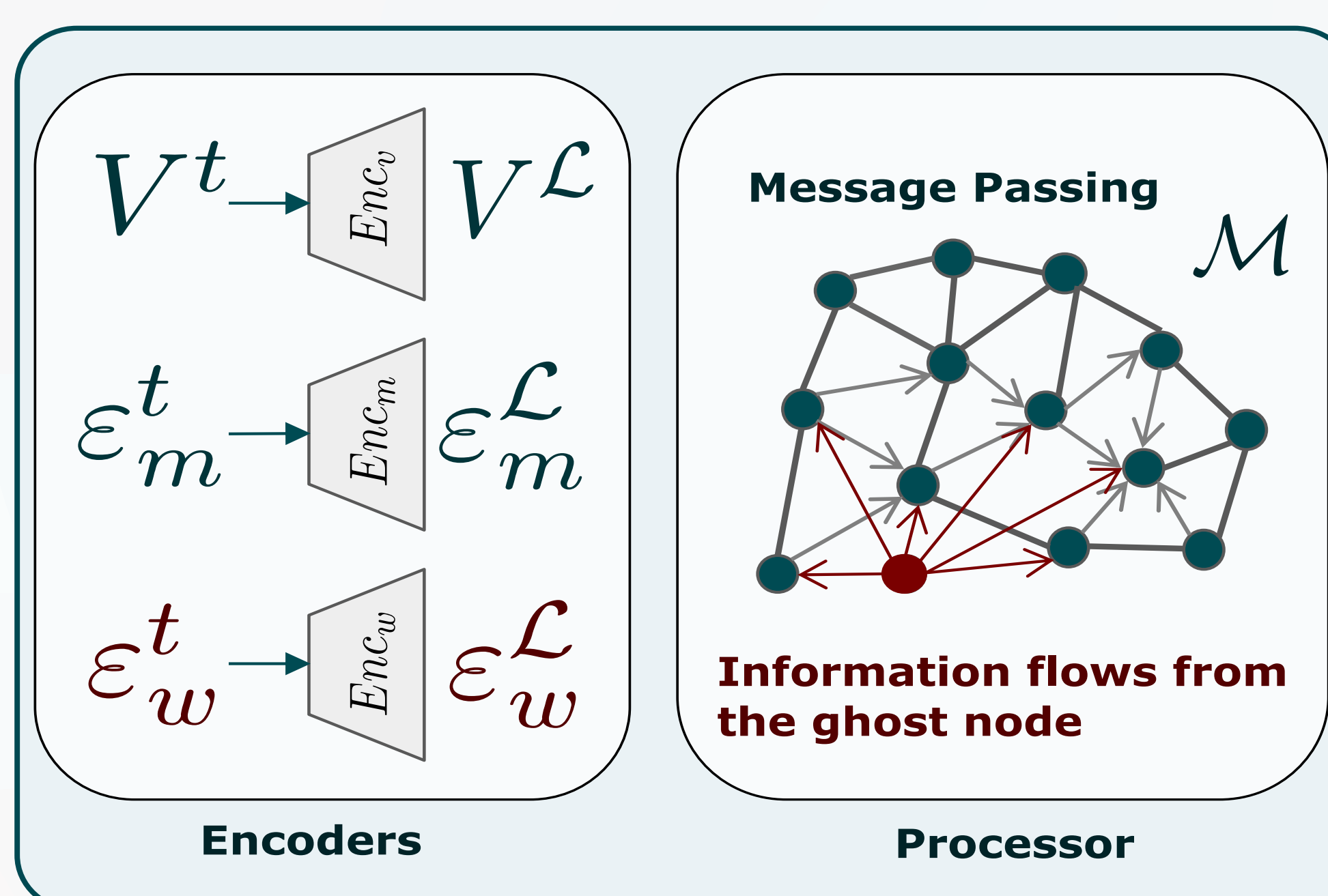
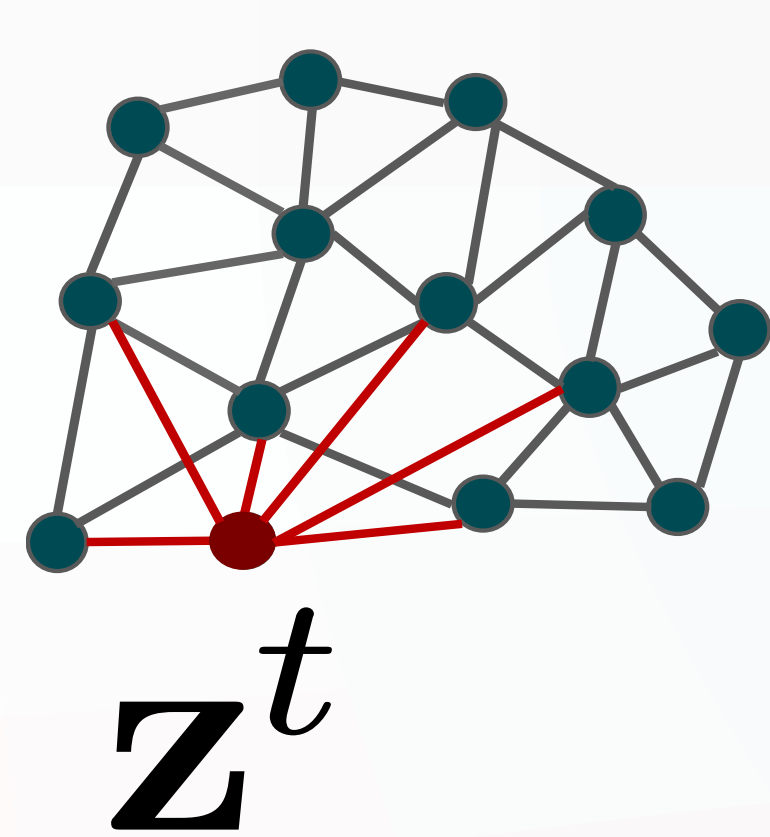
$$\mathbf{L}_i(\mathbf{z}_i) \frac{\partial s_i}{\partial \mathbf{z}_i} = 0$$

$$\mathbf{M}_i(\mathbf{z}_i) \frac{\partial \mathbf{e}_i}{\partial \mathbf{z}_i} = 0$$

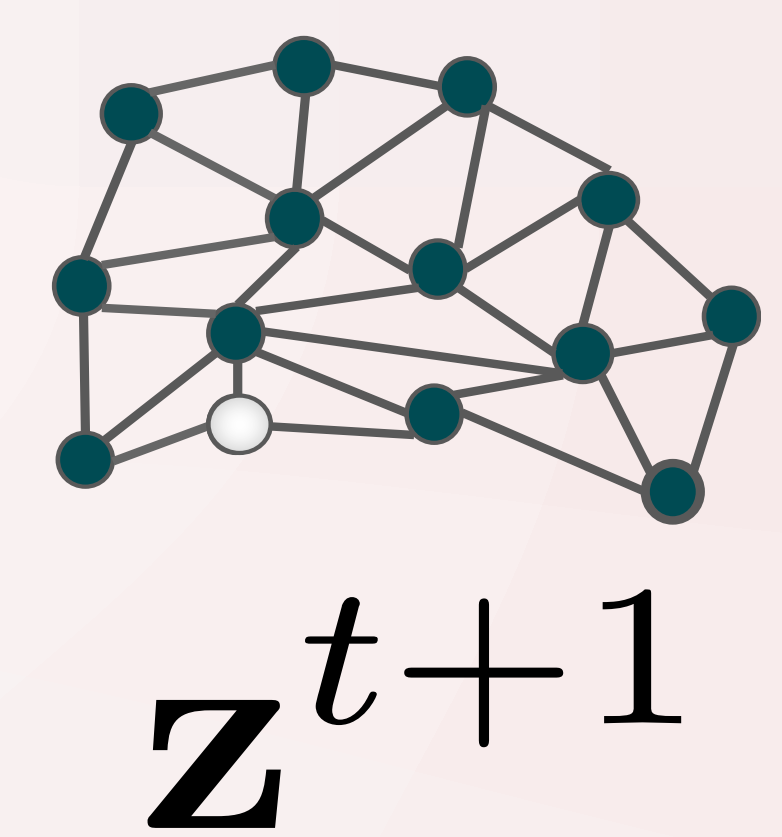
Degeneracy  
Conditions

## Forward pass:

$\mathbf{V}^t =$  Nodal Embeddings  
 $\boldsymbol{\varepsilon}^t =$  Edge Embeddings



## Net prediction

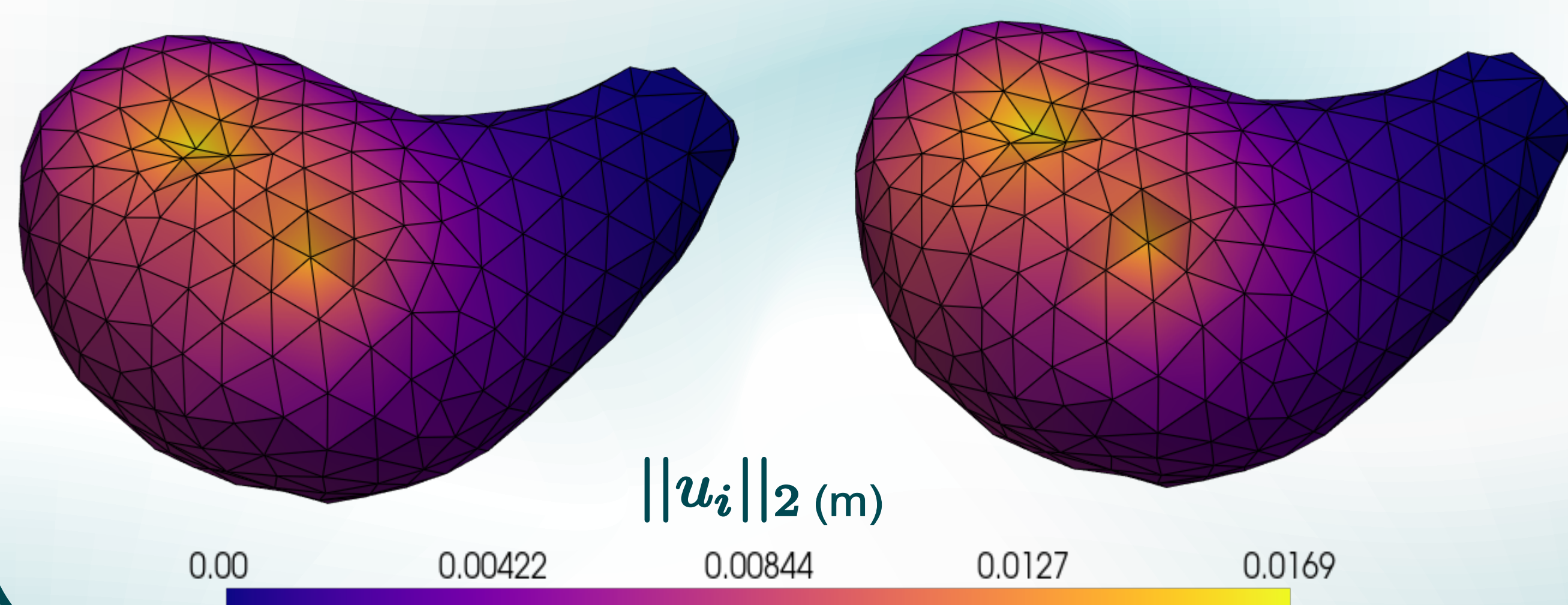


## Results and discussion:

Highly accurate predictions with high robustness

Ground Truth

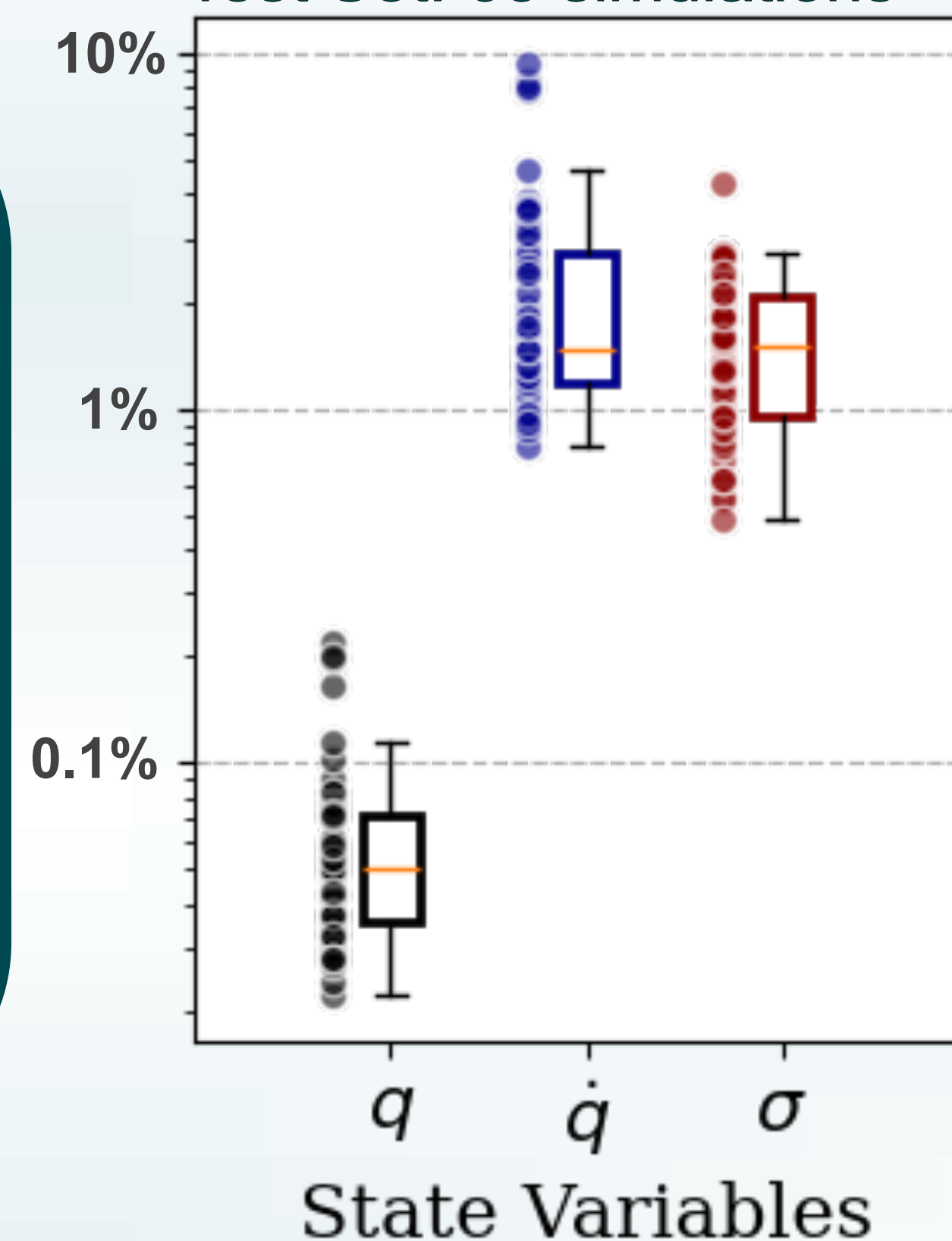
Prediction



Unseen load condition at inference!

## RRMSE Boxplot

Test Set: 63 simulations



## References

- [1]. HERNANDEZ, QUERCUS, et al. Thermodynamics-informed graph neural networks. arXiv preprint arXiv:2203.01874, 2022.
- [2]. PFAFF, Tobias, et al. Learning Mesh-Based Simulation with Graph Networks. arXiv preprint arXiv:2010.03409, 2021.
- [3]. MOYA, BEATRIZ, et al. Computational Sensing, Understanding, and Reasoning: An Artificial Intelligence Approach to Physics-Informed World Modeling. Archives of Computational Methods in Engineering, 2023, 1-18.
- [4]. TIERZ, A, et al. Graph Neural Networks Informed Locally by Thermodynamics. Preprint, 2024.

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Instituto Universitario de Investigación en Ingeniería de Aragón  
Universidad Zaragoza