XIII JORNADA DE JÓVENES INVESTIGADORES/AS DEL I3A

GRAPH NEURAL NETWORKS INFORMED LOCALLY BY THERMODYNAMICS

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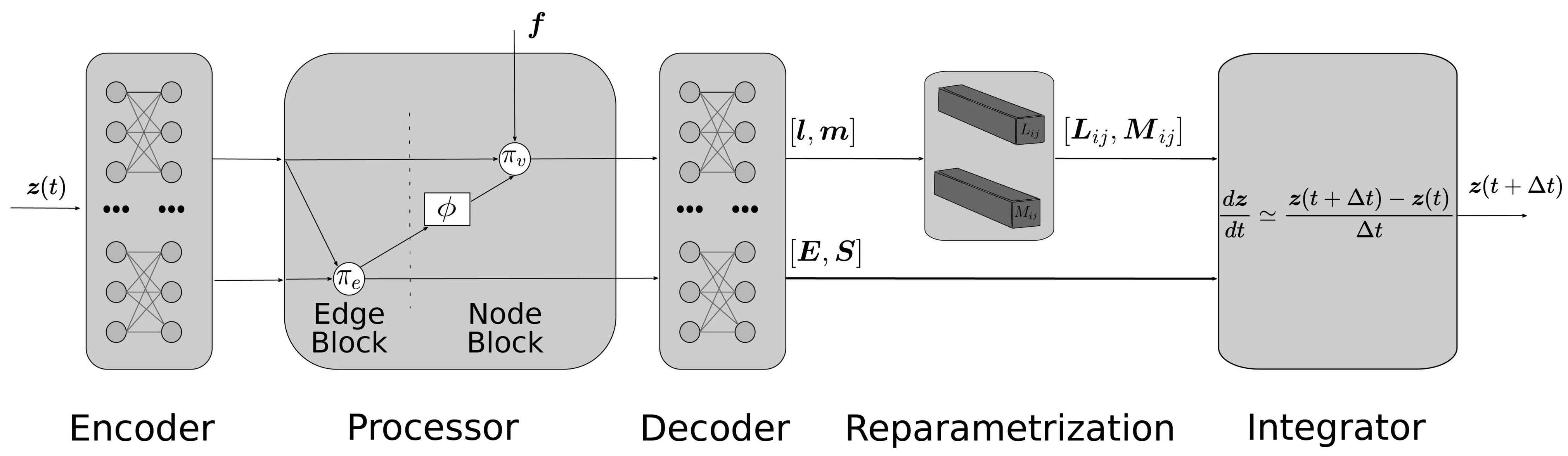
PROBLEM

- Most neural networks are black boxes and lack of interpretability
- We introduce basic physics knowledge learn[1] a general dynamic system from, either conservative or dissipative
- Find a generalizable method for different domain dependet problems with thousands of nodes

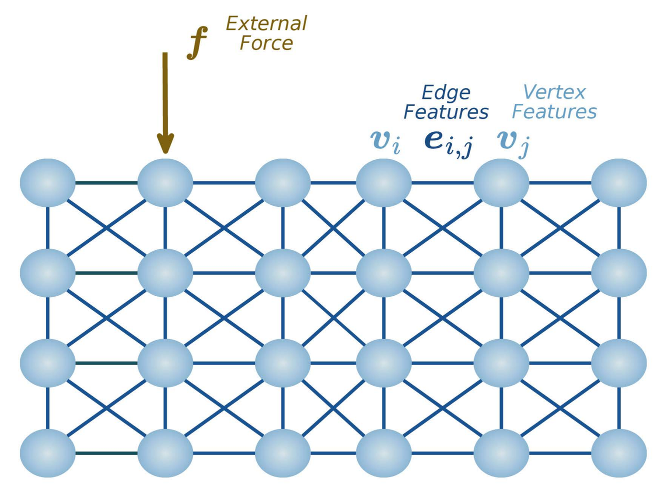


METHODS

- Inductive bias:

Metriplectic: We learn the GENERIC[23] structure of the problem, base on thermodynamics
Geometric: The neural network[4] perform calculations over the graph of the system to habdle non-Euclidean interactios

- A **local** implementation of thermodynamics-informed GNNs



GENERIC

$$\dot{\mathbf{z}} = \mathbf{L}(\mathbf{z})\frac{\partial E}{\partial \mathbf{z}} + \mathbf{M}(\mathbf{z})\frac{\partial S}{\partial \mathbf{z}}$$

Degeneracy conditions:

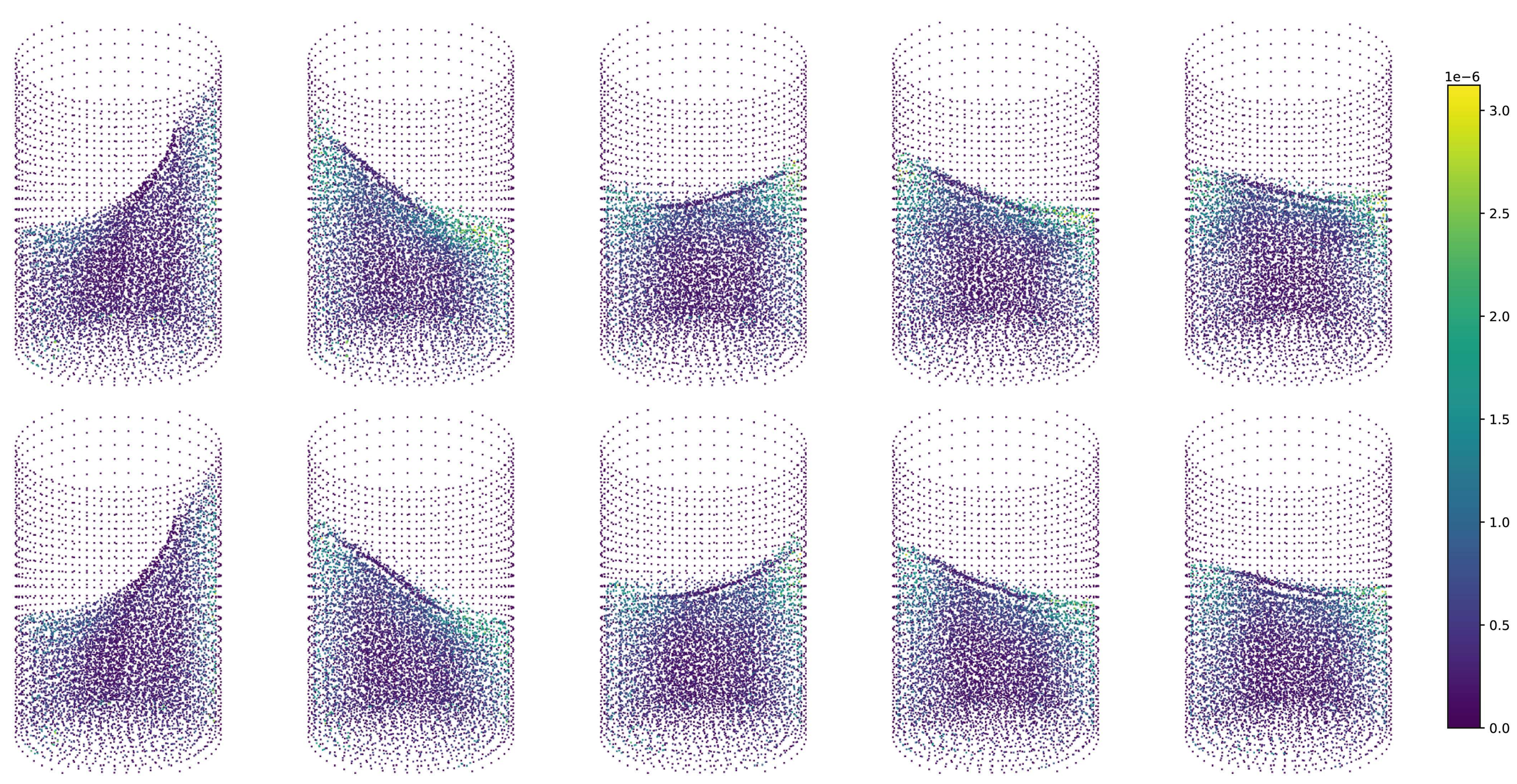
$$\mathbf{L}(\mathbf{z})\frac{\partial S}{\partial \mathbf{z}} = \mathbf{0} \qquad \mathbf{M}(\mathbf{z})\frac{\partial E}{\partial \mathbf{z}} = \mathbf{0}$$

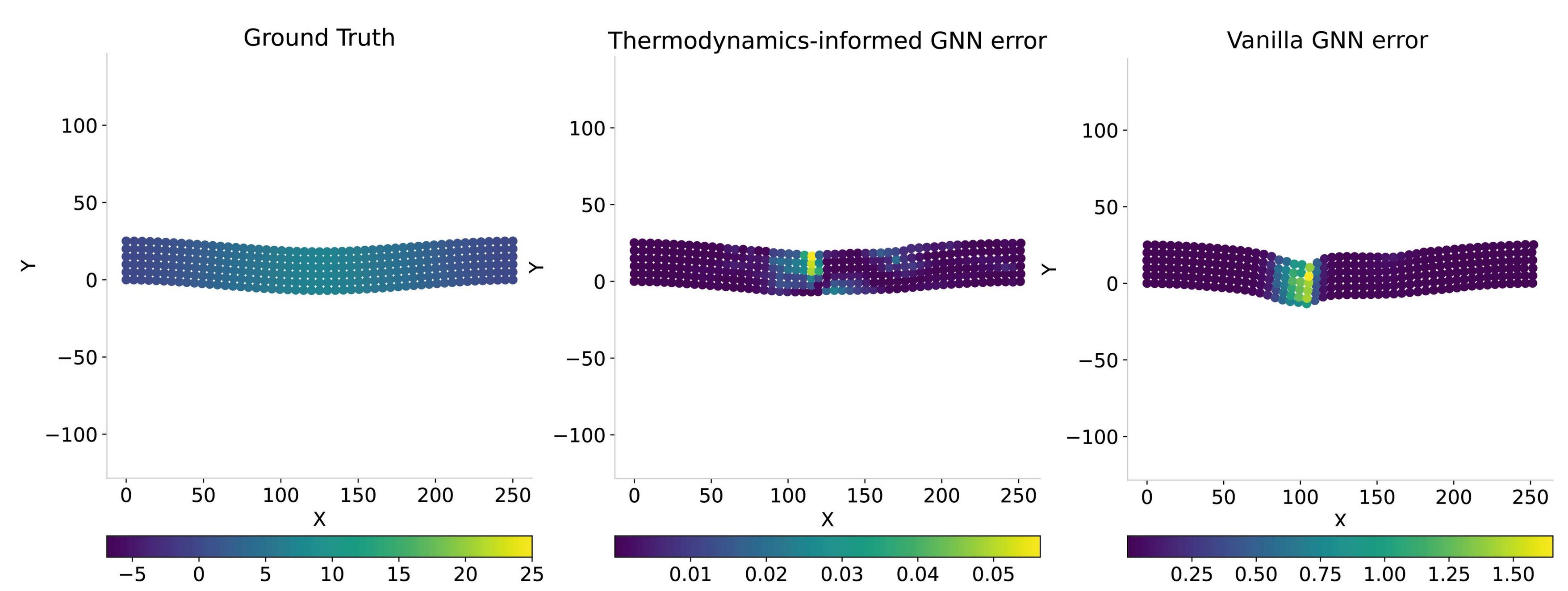
Local implementation of GENERIC

$$\dot{\mathbf{z}}_i = \mathbf{L}_i(\mathbf{z}_i)\frac{\partial e_i}{\partial \mathbf{z}_i} + \mathbf{M}_i(\mathbf{z}_i)\frac{\partial s_i}{\partial \mathbf{z}_i} - \sum_{j}^{\mathbf{n}_{\mathbf{neigh}}}\left[\mathbf{L}_{ij}(\mathbf{z}_j)\frac{\partial e_j}{\partial \mathbf{z}_j} + \mathbf{M}_{ij}(\mathbf{z}_j)\frac{\partial s_j}{\partial \mathbf{z}_j}\right]$$

Degeneracy conditions at particle level:

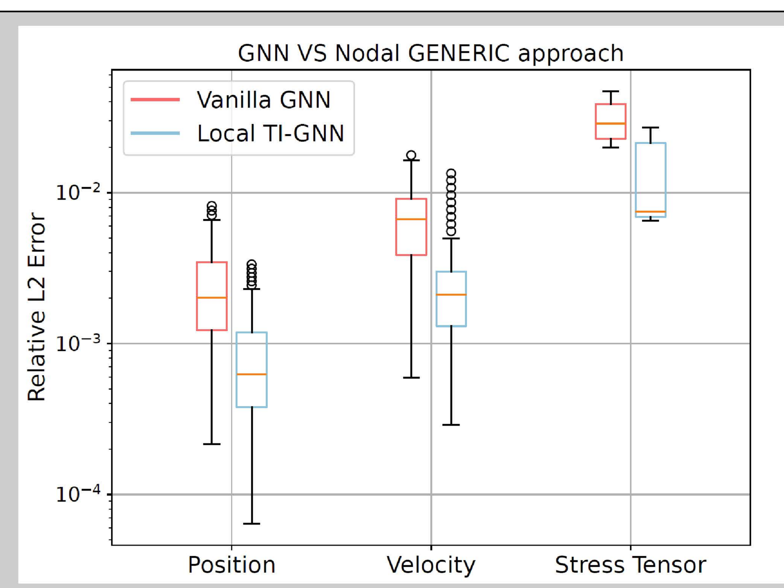
$$\mathbf{L}_i(z_i)\frac{\partial S_i}{\partial z_i} = 0 \quad \mathbf{M}_i(z_i)\frac{\partial E_i}{\partial z_i} = 0$$





RESULTS

- The introduction of local thermodynamic biases into graph neural networks enhances prediction accuracy and maintains computational efficiency, crucial for large-scale systems.
- Our method accelerates processing time by at least an order of magnitude compared to traditional methods, demonstrating both practical applicability and effectiveness.
- Strong generalization capabilities are observed, with accurate predictions on diverse examples, including beams clamped at both ends.



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RESULTS HERE!

REFERENCES

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