

# Flow estimation around arbitrary geometries by thermodynamics-informed neural networks

C. Bermejo-Barbanjo<sup>1</sup>, A. Badías<sup>1,2</sup>, D. González<sup>1</sup>, F. Chinesta<sup>3,4</sup>, E. Cueto<sup>1</sup><sup>1</sup>ESI Group-UZ Chair of the National Strategy on Artificial Intelligence, Aragon Institute of Engineering Research (I3A), Universidad de Zaragoza<sup>2</sup>ETSIAE, Universidad Politécnica de Madrid<sup>3</sup>ESI Group Chair, PIMM Lab, Arts et Métiers Institute of Technology<sup>4</sup>CNRS @CREATE LTD, Singapore

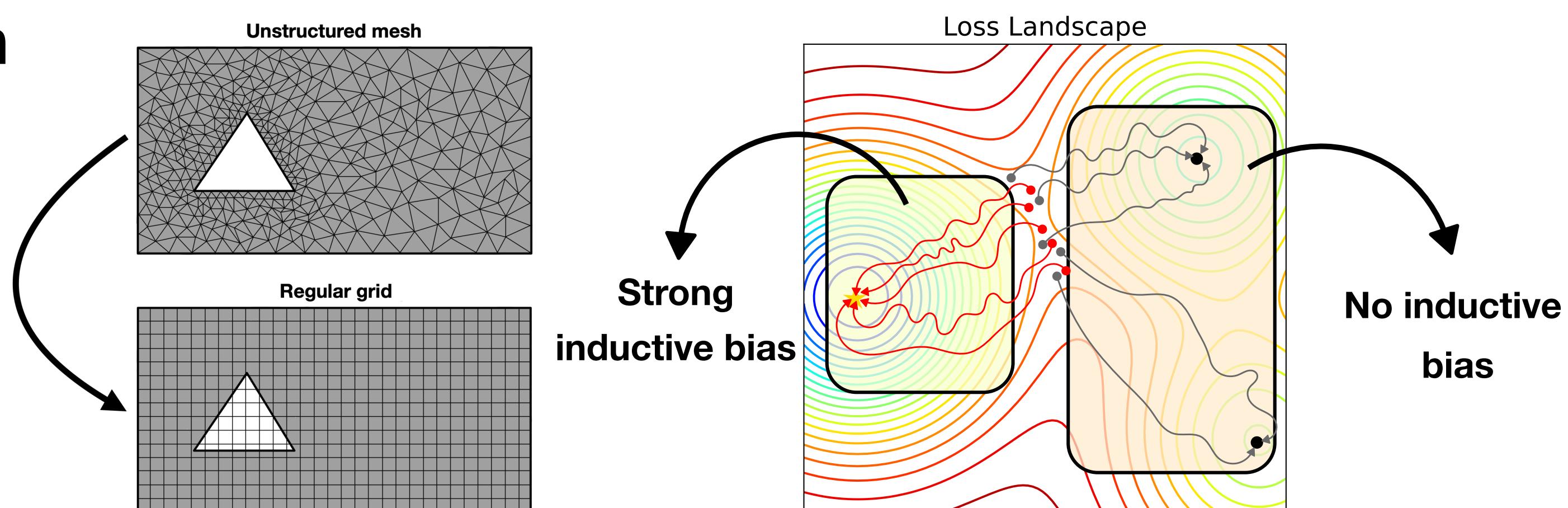
## INTRODUCTION

- Complex dynamic systems → High computational cost
- Digital twins, AR, VR: need for real-time predictions
- Machine learning approaches
  - + Very fast predictions
- Lack of physics
- Solution: deep learning + physics guidance

## METHODS

### Database Generation

- Unsteady flow over a 2D primitive geometries
- Simulations run in **OpenFOAM**<sup>1</sup>
- Post-processing:
  - Unstructured mesh to grid



## Deep Learning Framework

### 1 AAE - Adversarial Autoencoder<sup>2</sup>

- Learns a low dimensional manifold

### 2 SPNN - Structure Preserving Neural Network<sup>3</sup>

- Predicts the dynamical evolution of the system
- Applies the metriplectic bias - **GENERIC** Formalism

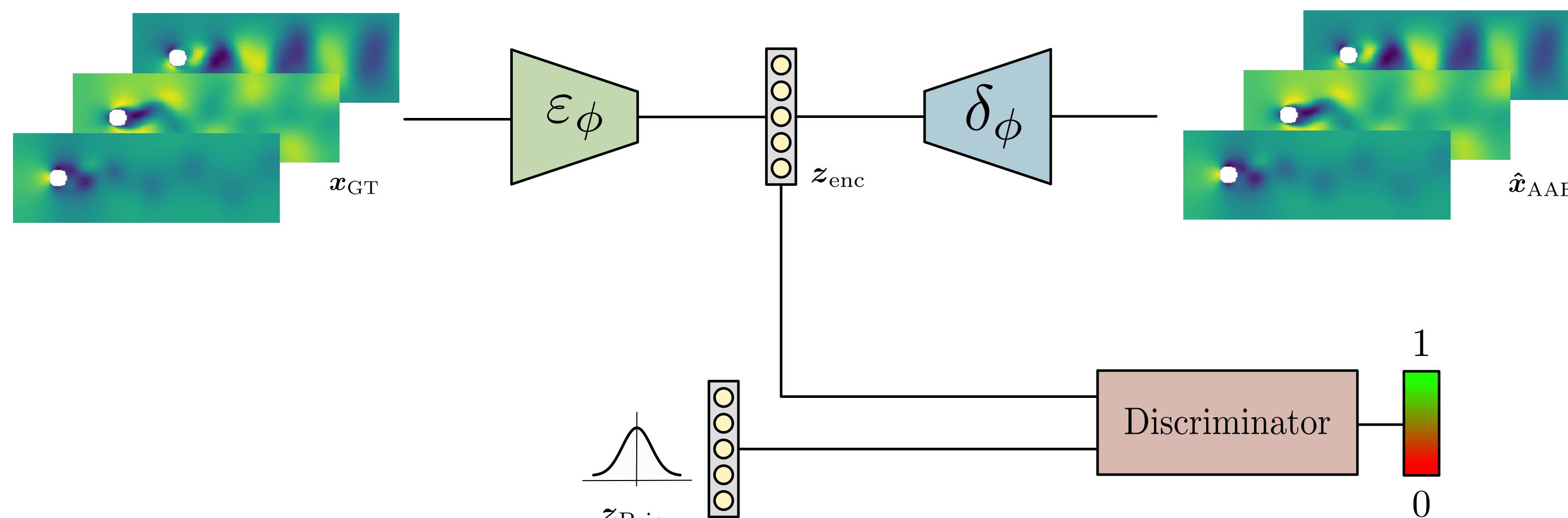
### General Equation for Non-Equilibrium

#### Reversible-Irreversible Coupling (GENERIC)<sup>4,5</sup>

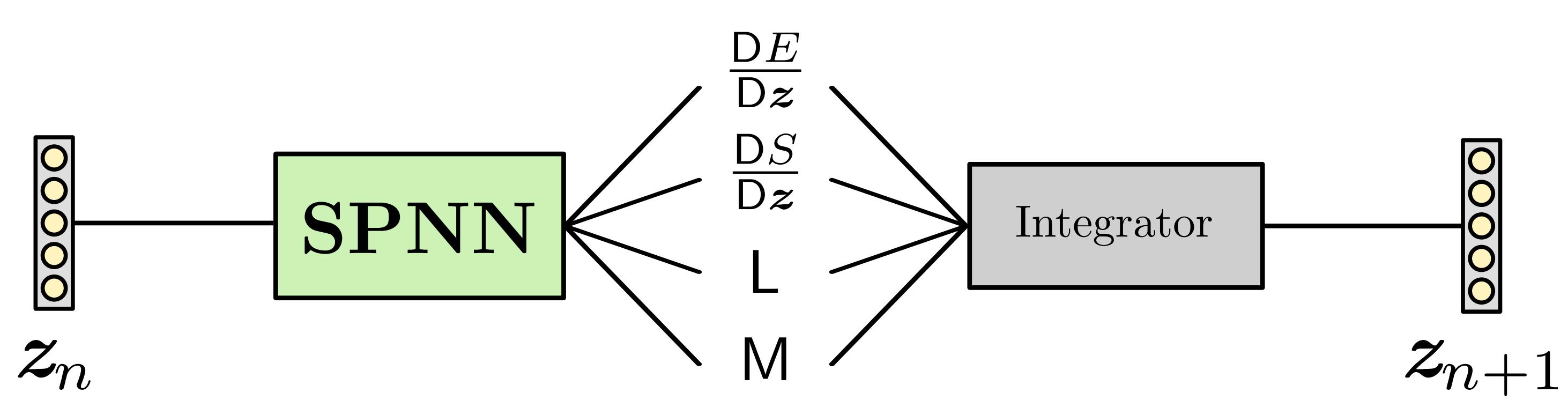
$$\frac{d\mathbf{z}}{dt} = \mathbf{L} \frac{\partial E}{\partial \mathbf{z}} + \mathbf{M} \frac{\partial S}{\partial \mathbf{z}} \quad \left\{ \begin{array}{l} \mathbf{L} \frac{\partial S}{\partial \mathbf{z}} = 0 \Rightarrow \frac{dE}{dt} = 0 \\ \mathbf{M} \frac{\partial E}{\partial \mathbf{z}} = 0 \Rightarrow \frac{dS}{dt} \geq 0 \end{array} \right.$$

Symplectic manifold → Metriplectic manifold<sup>6</sup>

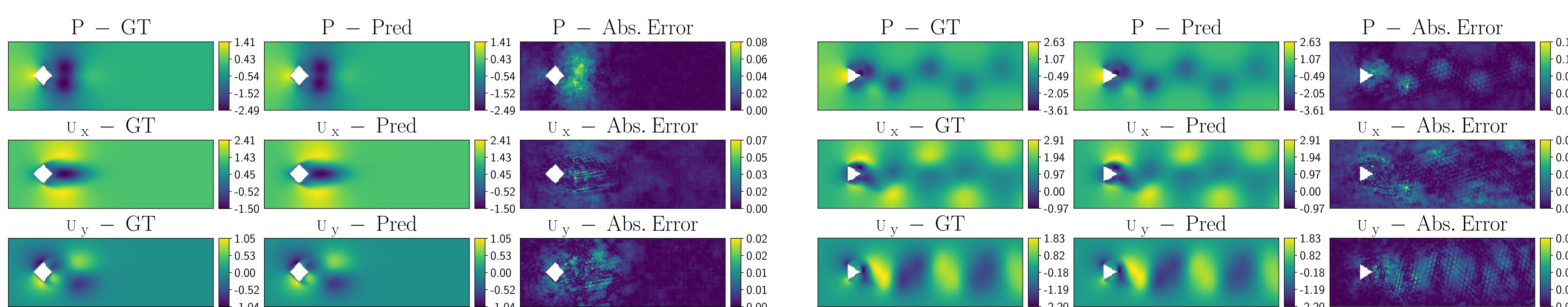
### 1 Adversarial Autoencoder



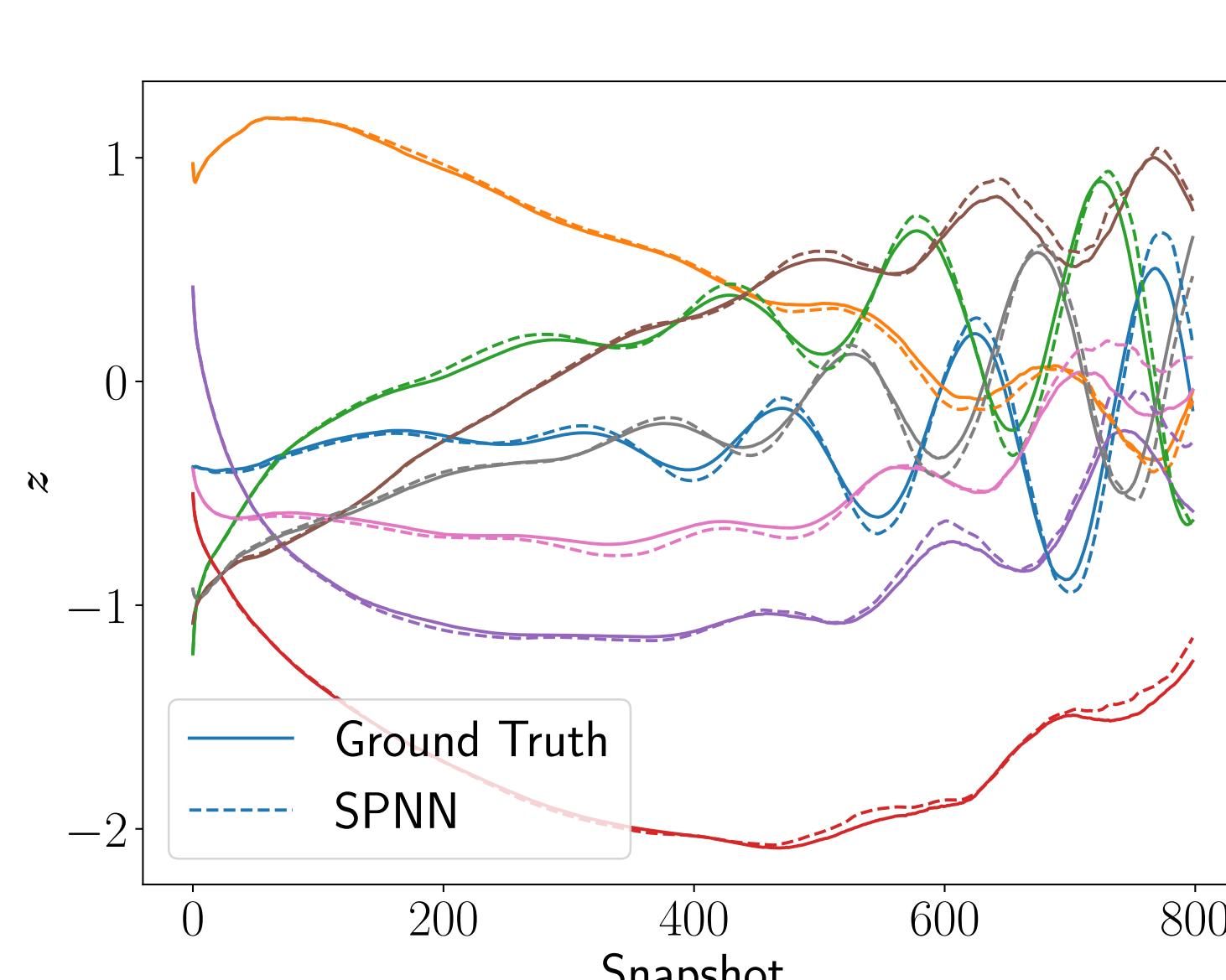
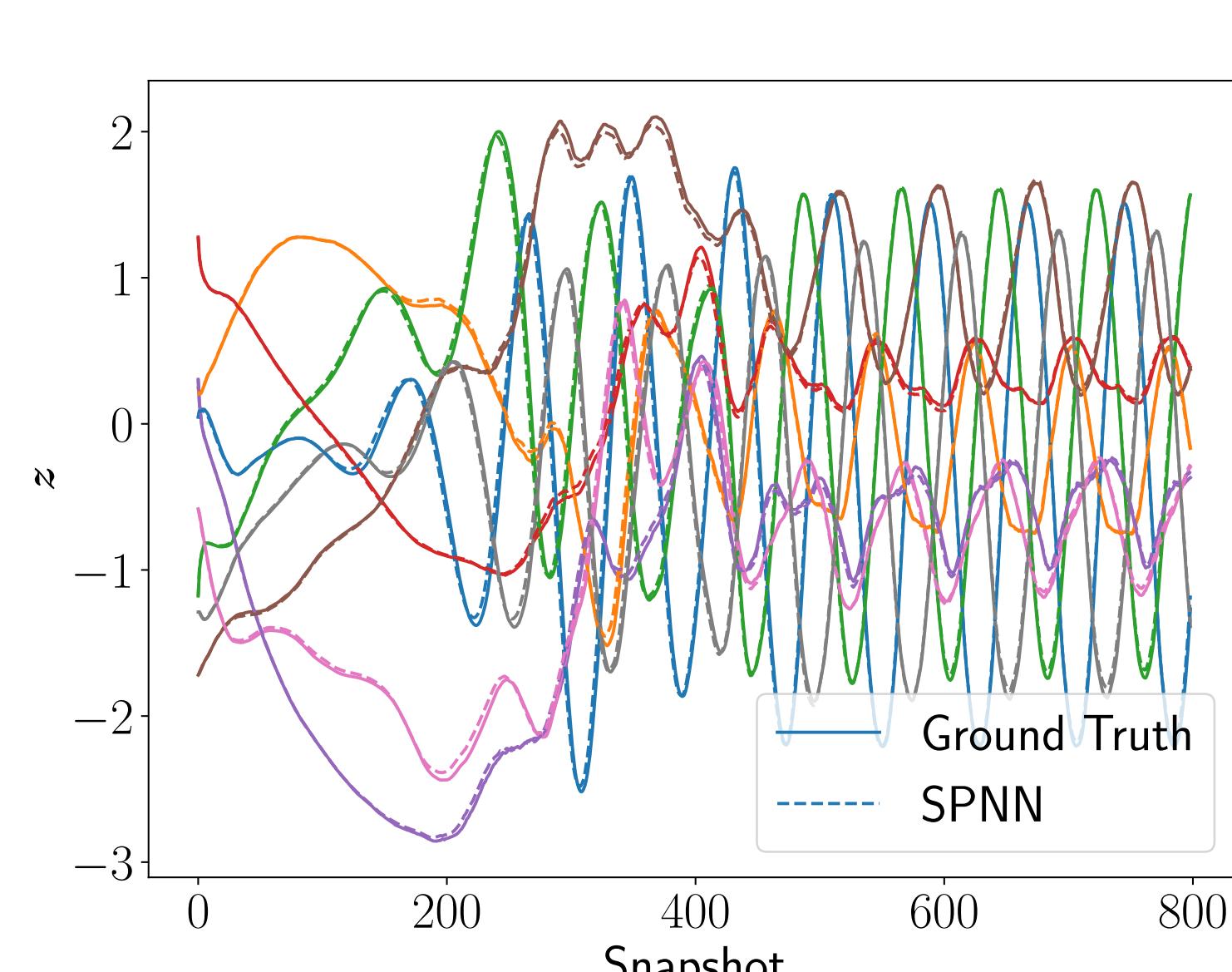
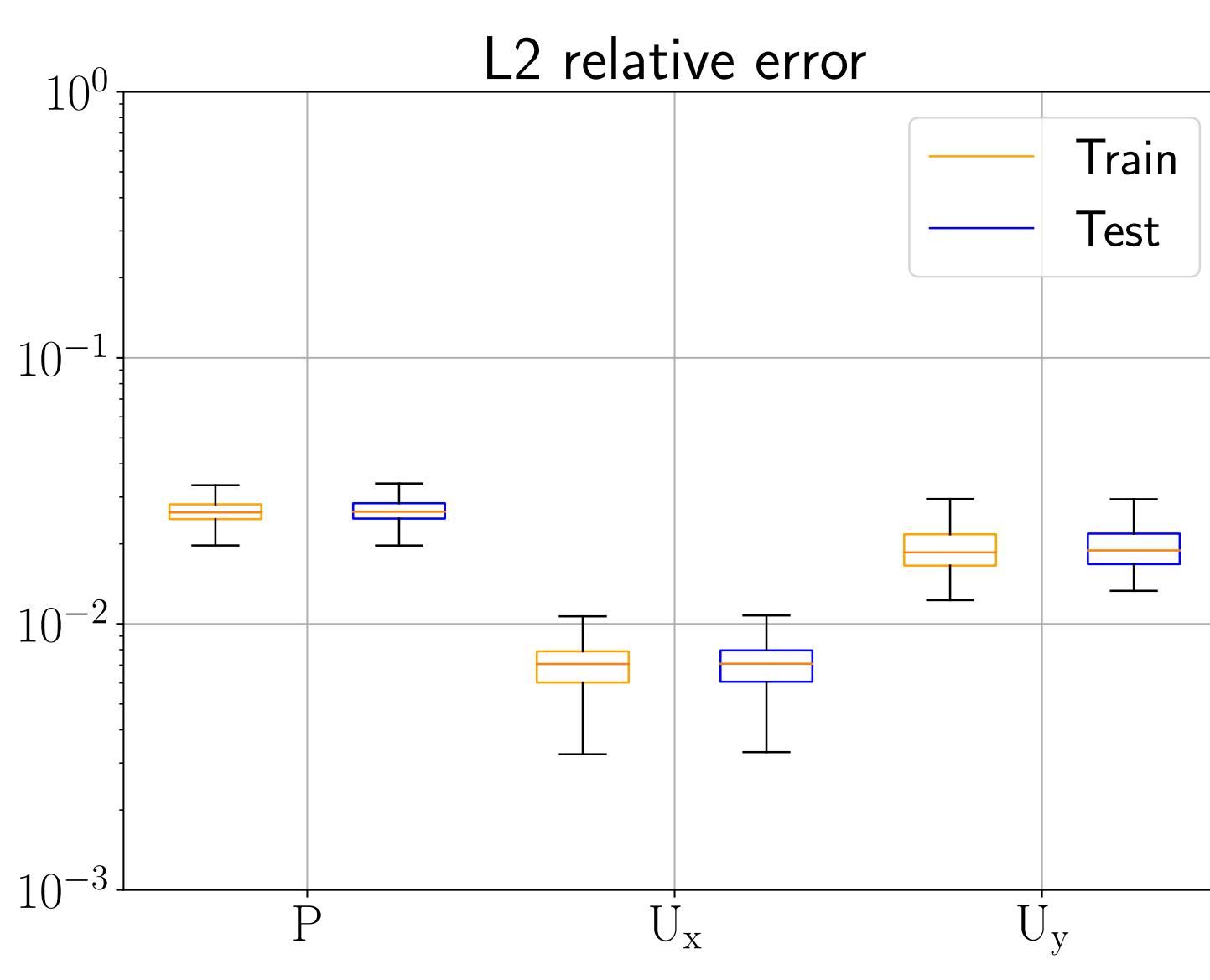
### 2 Structure Preserving Neural Network



## RESULTS



VIDEOS  
HERE!



## CONCLUSIONS

- Successful codification of the flow achieved by the **AAE**
- Thermodynamics-based biases help to improve robustness and generalization

## FUTURE WORK

- Apply metriplectic and geometric biases together - **GNN**



cbberbarbanjo@unizar.es

@cberbarbanjo

github.com/cberbarbanjo

amb.unizar.es/people/carlos-bermejo-barbanjo

## References

- WELLER, H.G. et al. (1998). A tensorial approach to computational continuum mechanics using object-oriented techniques, *Computers in Physics*, Vol. 12, NO. 6.
- MAKHZANI, A. et al. (2015). Adversarial autoencoders. *ArXiv preprint*. arXiv:1511.05644.
- HERNÁNDEZ, Q., et al. (2021). Structure-preserving neural networks. *Journal of Computational Physics*, vol. 426, p. 109950.
- GRMELA, M. and ÖTTINGER, H.C. (1997). Dynamics and thermodynamics of complex fluids. I. Development of a general formalism. *Physical Review E* 56. 56(6), p.6620.
- ÖTTINGER, H.C. and GRMELA, M. (1997). Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism. *Physical Review E* 56. 56(6), p.6633.
- MORRISON, P.J. (1986). A paradigm for joined Hamiltonian and dissipative Systems. *Physica D: Nonlinear Phenomena*. 18(1-3), 410 - 419.