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X JORNADA DE JÓVENES INVESTIGADORES DEL I3A

LEARNING PHYSICS WITH GRAPHS

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INTRODUCTION

Computational modelling has become a standard tool in a wide variety of scientific fields, in order to simulate reality phenomena and predict its future behaviour.

The aim of this work is to learn **physical simulators** with the correct mathematical structure using graph-based deep learning.

METHODS

We take advantage of two inductive biases [1]:

Geometric structure: We are able to exploit the geometric constraints of the system by performing computations over graphs based on the nodal connectivities. This enables the algorithm to learn more complex interactions, even in non-Euclidean manifolds [2].

Metriplectic structure: The time prediction is achieved via a thermodynamically consistent integrator based on the GENERIC formalism [3]. It divides the system into conservative dynamics, related to Hamiltonian mechanics, and dissipative dynamics.

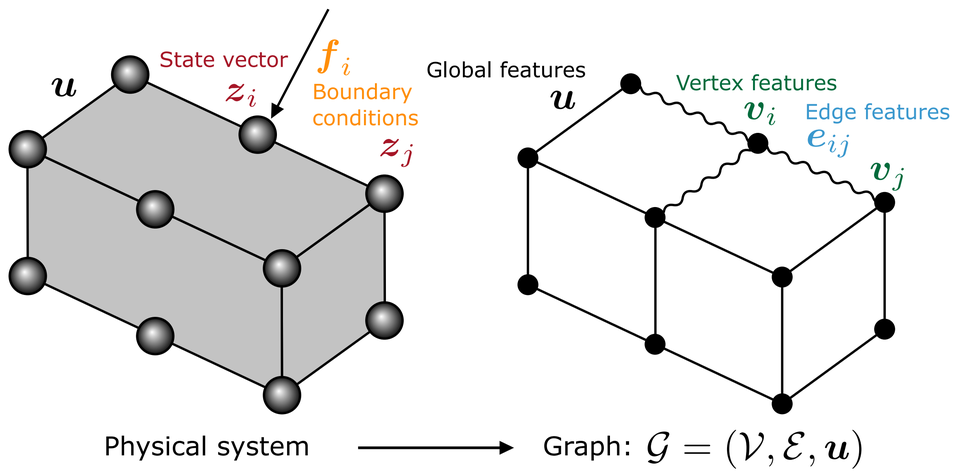
$$\frac{d\boldsymbol{z}}{dt} = \boldsymbol{L}\frac{\partial E}{\partial \boldsymbol{z}} + \boldsymbol{M}\frac{\partial S}{\partial \boldsymbol{z}} \qquad \boldsymbol{L}\frac{\partial S}{\partial \boldsymbol{z}} = \boldsymbol{M}\frac{\partial E}{\partial \boldsymbol{z}} = 0$$

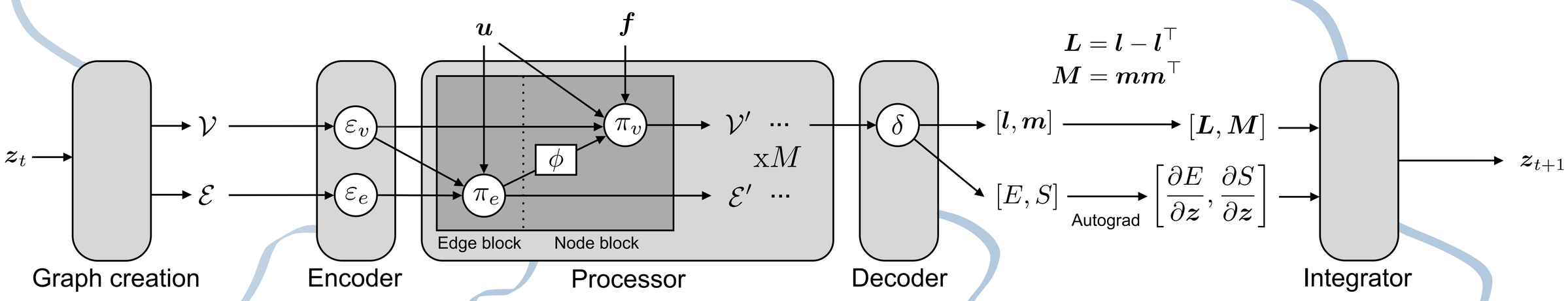
Conservative term:
E: Energy
$\boldsymbol{L}$: Poisson operator

Dissipative term:
S: Entropy
$\boldsymbol{M}$: Friction operator

Degeneracy conditions: Ensure the fullfulment of the first and second laws of thermodynamics.

1 The physical magnitudes of the domain are converted to vertex (nodal properties) and edge (interactions) **feature vectors**.





2 We use an encoder to embed the feature vectors into higher-dimensional **latent vectors**.

3 The processor computes the update of the latent vectors based on the node connectivity in a **message passing** scheme [4].

4 The decoder computes for each particle the **GENERIC operators** and **potentials**. The symmetric and positive semi-definite conditions are imposed by construction.

$$\frac{d\boldsymbol{z}}{dt} \simeq \frac{\boldsymbol{z}_{t+1} - \boldsymbol{z}_t}{\Delta t}$$

5 The state vector is updated using the **GENERIC equation** and a simple forward-Euler scheme.

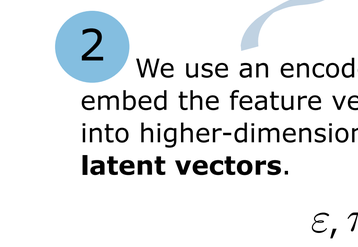
ε, π, δ: MLPs with shared parameters for all nodes
ϕ: Aggregation function, permutation invariant (sum)
M: Processor sequential cores with residual connections

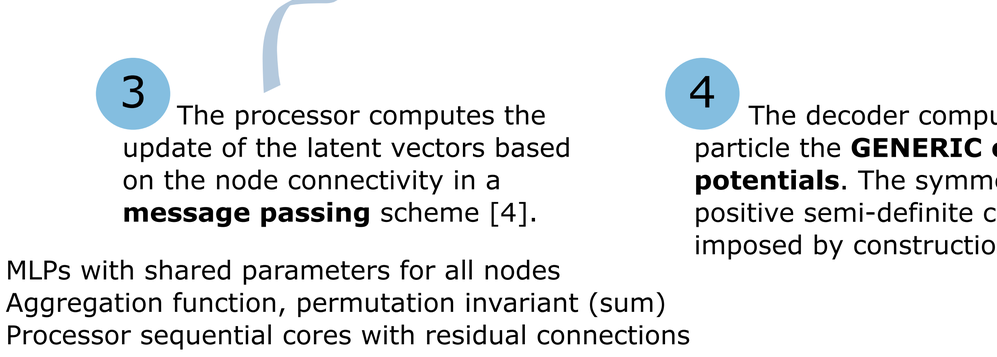
RESULTS

Two multiparametric fluid and solid mechanic examples are tested with the proposed method in a **rollout** scheme. The algorithm is compared in an ablation study with two previous methods: GNN [5] (no metriplectic bias) and SPNN [6] (no geometric bias).

Couette flow: Olrody-B fluid with varying Reynolds and Weissemberg numbers.

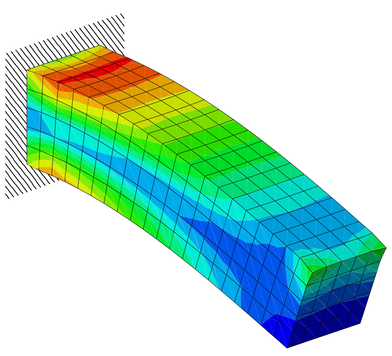
$\boldsymbol{z}_i = [\boldsymbol{q}_i, v_i, e_i, \tau_i] \qquad \boldsymbol{u} = [\mathrm{Re}, \mathrm{We}]$

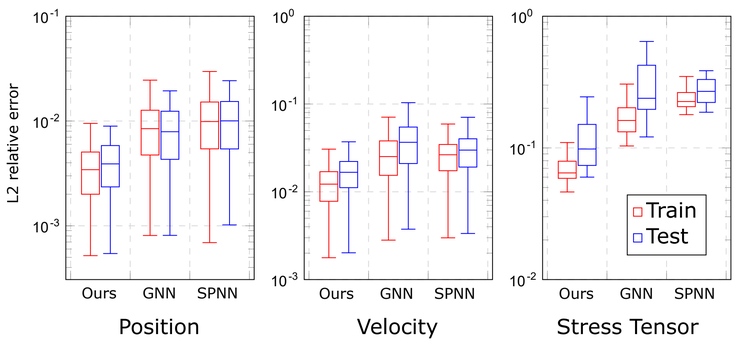




Bending beam: Viscoelastic solid with varying load modulus and position.

$\boldsymbol{z}_i = [\boldsymbol{q}_i, \boldsymbol{v}_i, \boldsymbol{\sigma}_i] \qquad \boldsymbol{f}_i = [\boldsymbol{F}_i]$





CONCLUSIONS

We have presented a method to predict physics from data with a graph-based deep learning algorithm, which takes advantage of the geometric properties of the system.

The addition of the correct metriplectic structure also ensures the thermodynamical consistency of the results, satisfying the energy conservation and entropy inequality for dissipative systems.

This combined method of both inductive biases outperform the existing state of the art works, achieving consistent relative errors within **1%** in rollout test simulations.

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