Graph Neural Networks with Embedded Symmetries for Robust Computational Homogenization

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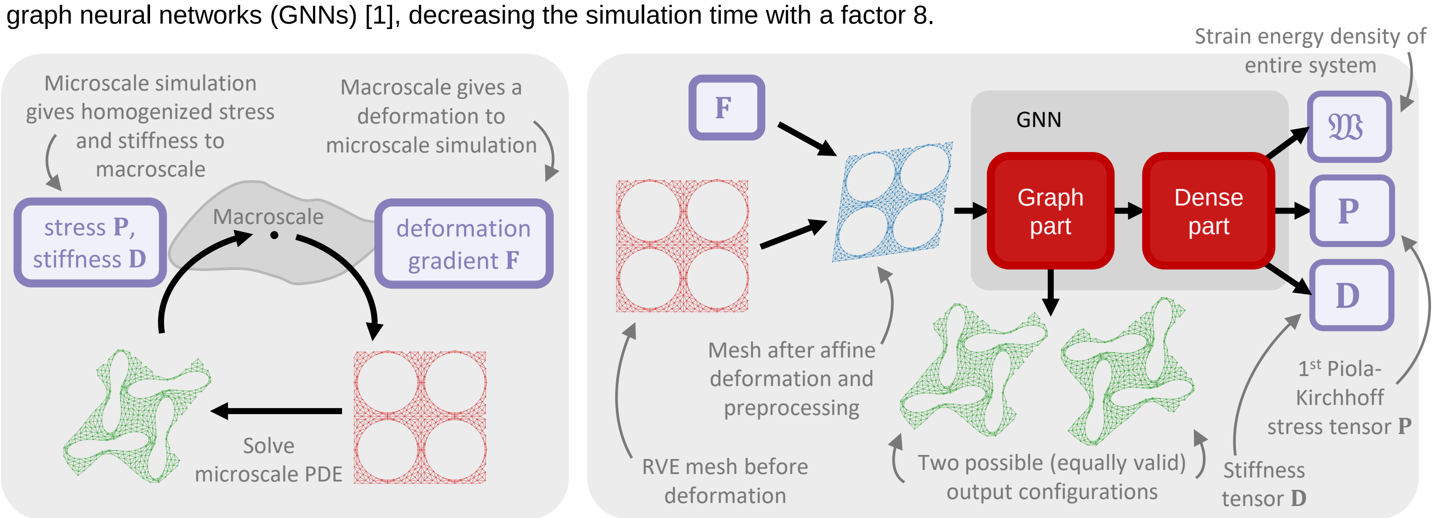
Introduction

Porous, flexible metamaterials are useful in soft robotics. To design these materials, the mechanical behavior needs to be modelled. Current computational homogenization of a periodic representative volume element (RVE) using the finite element method (FEM) is too slow to optimize the design. Therefore, a surrogate model, replacing FEM, is used to quickly simulate the mechanical behavior of the porous materials obtaining the stress $\mathbf{P}$ in the material and its stiffness $\mathbf{D}$, described by the deformation gradient $\mathbf{F}$. We create a newly developed surrogate model of the material behavior using graph neural networks (GNNs) [1], decreasing the simulation time with a factor 8.



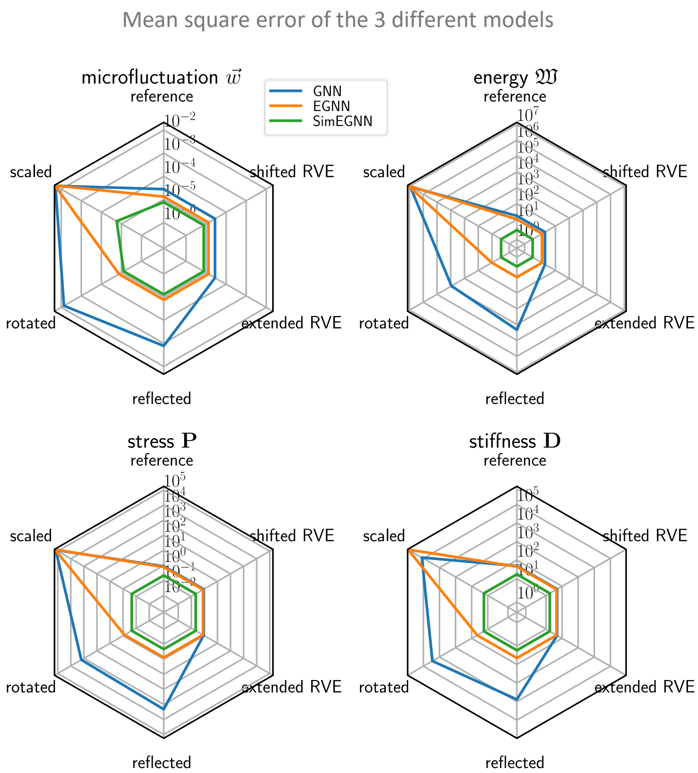
Incorporating symmetries

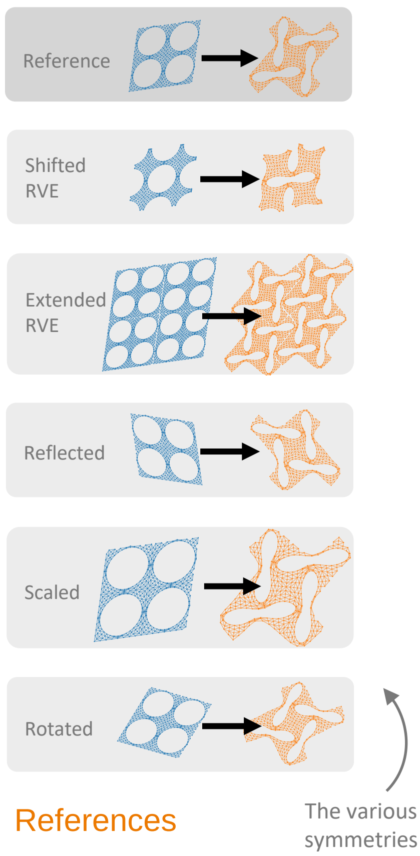
For optimal accuracy and efficiency, GNNs need to respect the right symmetries, such that the output transforms with the input in the correct way.

Results

Three models, with varying types of symmetries embedded, are compared. The model that respects all symmetries has the lowest mean squared error.

- **GNN**: periodicity
- **EGNN**: GNN plus rotation and reflection
- **SimEGNN**: EGNN plus scaling





Future work

Often the material can buckle in several different ways. To ensure the model can predict all valid solutions, a generative model will be used. We are also looking at geometrical parametrization of the input.

References

[1] Satorras, Vıctor Garcia, Emiel Hoogeboom, and Max Welling. "$E(n)$ equivariant graph neural networks." International conference on machine learning. PMLR, 2021.