Predicting plastic strain localization in porous solids using graph neural networks

Graphs&Data seminar

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TUDelft

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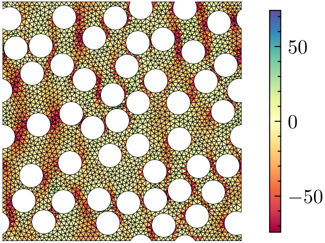
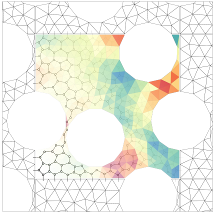
Eccomas 2024 - presenting GNNs to accelerate FEM simulations





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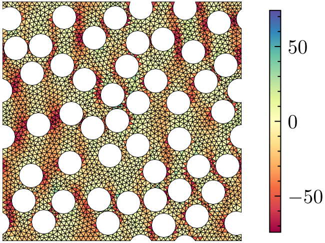
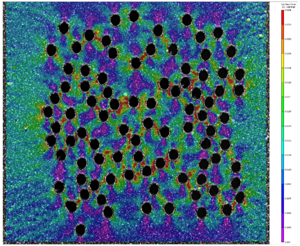
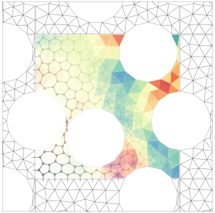
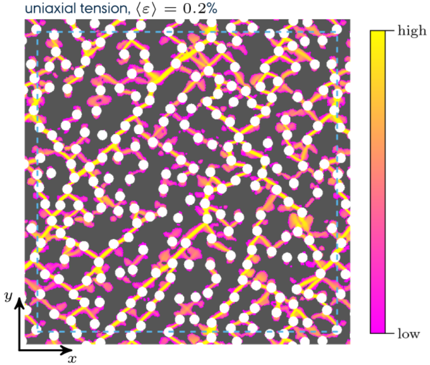






Their previous work:

For ductile solid materials, deformation localizes in shear bands.



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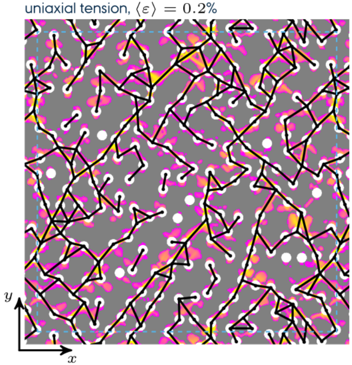
- Key observation: shear bands occur between porosities
- FEM simulations provide the plastic work rate w^p.

  A watershed algorithm on w^p connects nodes



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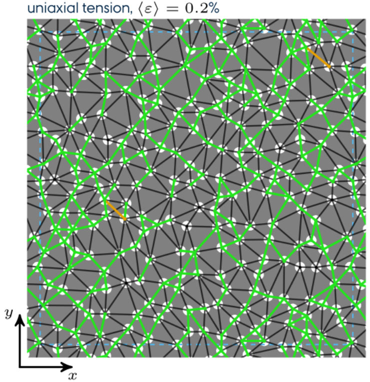
- Almost all links (99.5%) occur in a Delaunay network, where voids are represented as nodes



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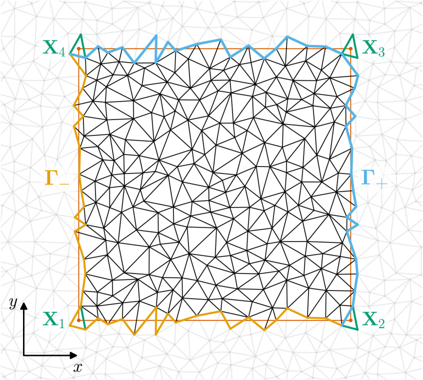
Instead of using FEM, model the Delaunay network as rigid blocks that only deform along boundaries.[1]
This can be formulated as a linear programming problem, which can be efficiently solved.



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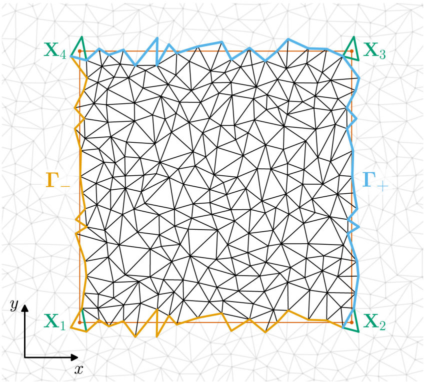

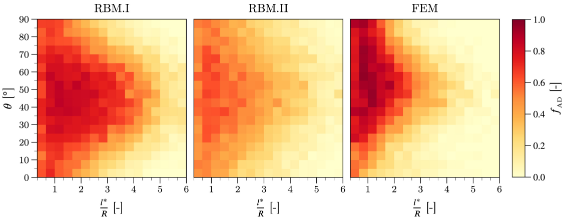

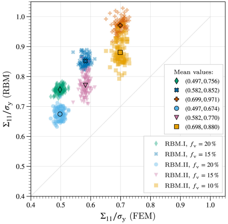

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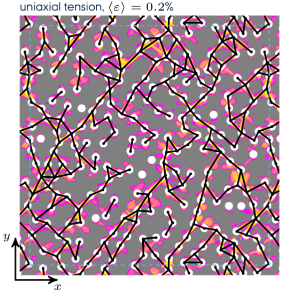
Can we use GNNs to increase the accuracy?

Work carried out by Rasmus B. Jakobsen and Tobias S. Kristensen as part of their MSc thesis at Aarhus University.

Objectives:

- Predict the shear band pattern
- Quantify the total rate of work



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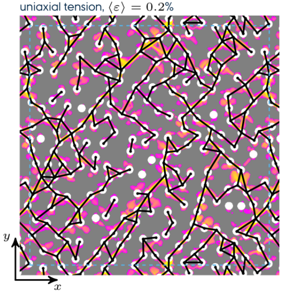

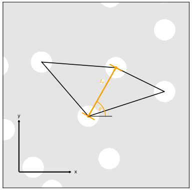

GNN setup:

- Delaunay triangulation as the graph
- Node features: -
- Edge features:
  - Edge length
  - Edge orientation w.r.t. load angle
- Target:
  - Edge scalar (plastic work rate $\dot{w}^p$)
- Data: 1200 simulations with random void distributions

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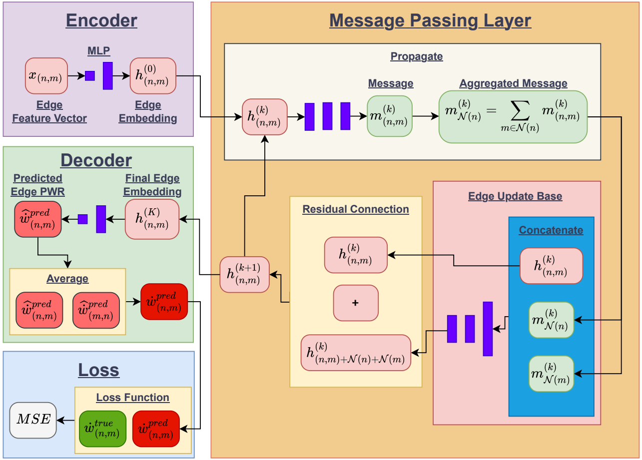
GNN architecture

Encode $\rightarrow$ Process $\rightarrow$ Decode procedure.

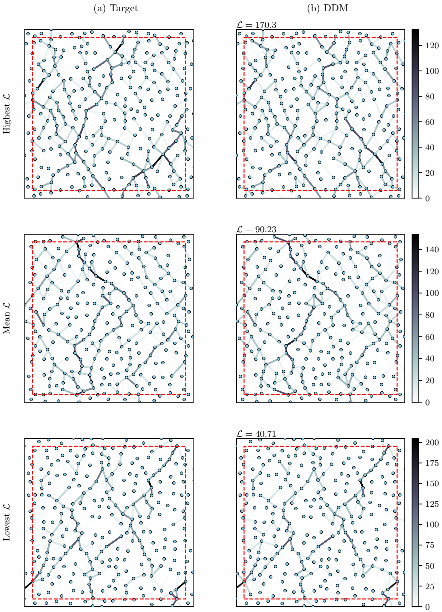
- No nodal embeddings



GNNs can accurately predict shear bands

Worst, median and best test sample.

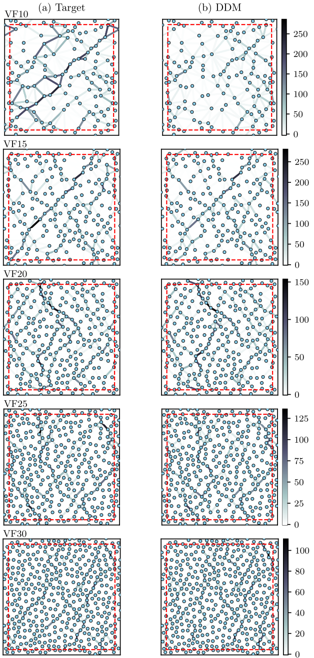
Edge opacity reflects their scalar quantity.



We cannot extrapolate to other void distributions

Reducing or increasing the void fraction worsens performance

Training only on $V_f = 20\%$.



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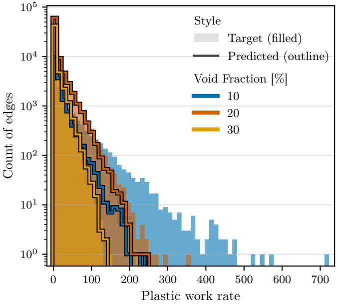

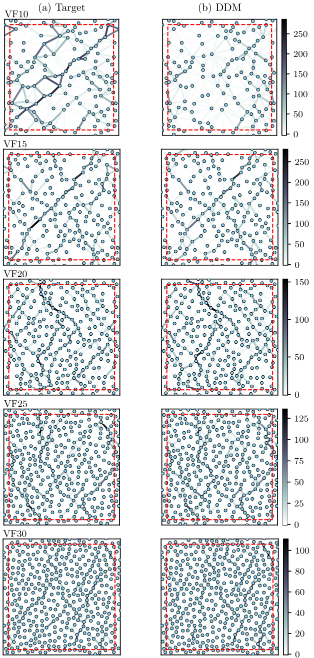

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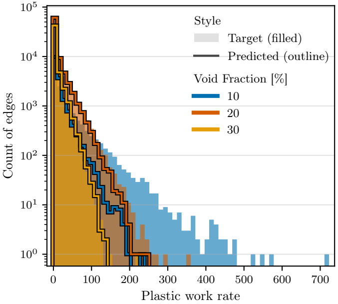
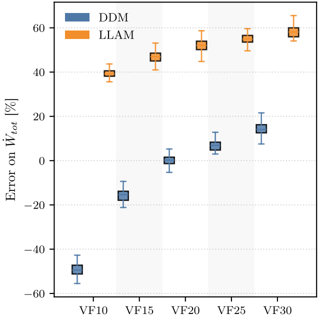
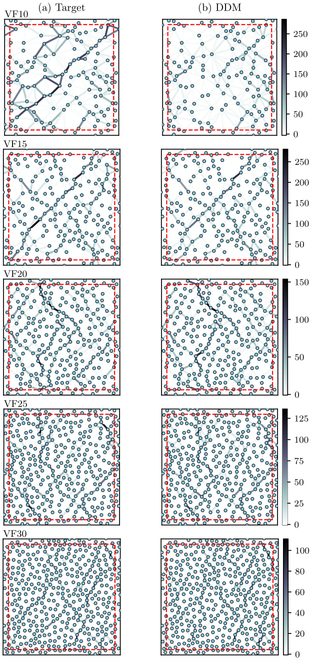






Hybrid model: using a physical prior

Additional edge feature: the physics-based prediction for $\dot{w}^p$.

$$\dot{w}^{pred}_{(n,m)} = \underbrace{\dot{w}^{LLAM}_{(n,m)}}_{\text{physical prior}} + \underbrace{GNN\left(\theta, l, \dot{w}^{LLAM}\right)}_{\text{corrector}} \tag{1}$$

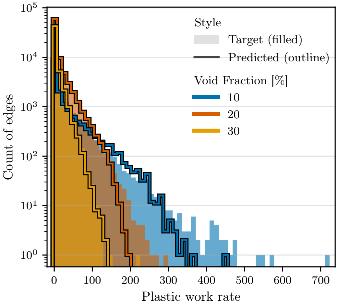
Change of loss function:

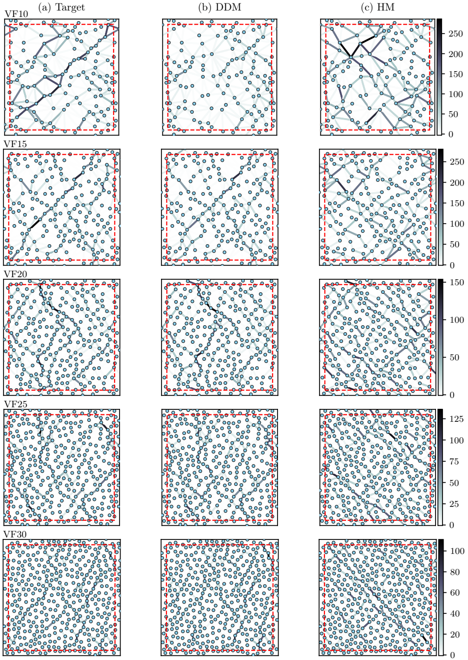
- The prior can give the right overall behavior, but with the wrong specific pattern
- A MSE loss comparing individual edges over-punishes this
- We therefore use the 2-Wasserstein loss, matching the overall distribution instead of specific edges

$$\mathcal{L}_{W_2^2} = \frac{1}{|\mathcal{E}|} \sum_{i=1}^{|\mathcal{E}|} \left(s_i^{\downarrow} - t_i^{\downarrow}\right)^2 \tag{2}$$

Hybrid model result in extrapolation:

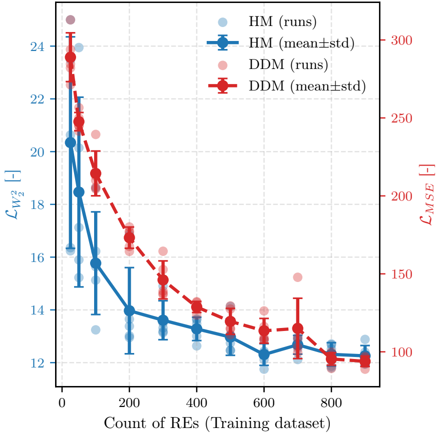
The hybrid model better follows the target distribution





The hybrid model requires less training data

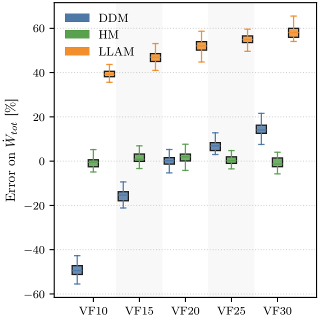
Learning curve:



Better extrapolation on the total work rate

Due to the physical prior, the hybrid model closely follows the total work rate when extrapolating.

Both HM and DDM are trained on $VF20$.



Conclusion

Two GNN models are explored:

- A data-driven GNN reproduces the shear band pattern
- Using a physical-prior reduces data requirements, and improves extrapolation capability

This enables predicting failure while accounting for a large number of voids

Future directions:

- Better handle cases dominated by a few edges with very high values (skewed distributions)
- Extend the approach beyond elastic-perfectly plastic materials