Novel geometric deep learning surrogate framework for non-linear finite element simulations

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MARIE CURIE ACTIONS

Motivation & Overview of the MAgNET Framework

Motivation

- High-fidelity computational models can be too slow for practical use, leading to the need for faster surrogate models.
- Deep learning techniques are being increasingly used to accelerate simulations, but struggle with larger and complex problems.

Solution

- A novel geometric deep learning framework for mesh based simulations.
- New neural network layers for graph-structured data such as meshes.

Implementation

- Proposed networks are trained on synthetic non-linear FEM datasets.
- Validated against state-of-the-art CNN U-Net framework [2, 3].

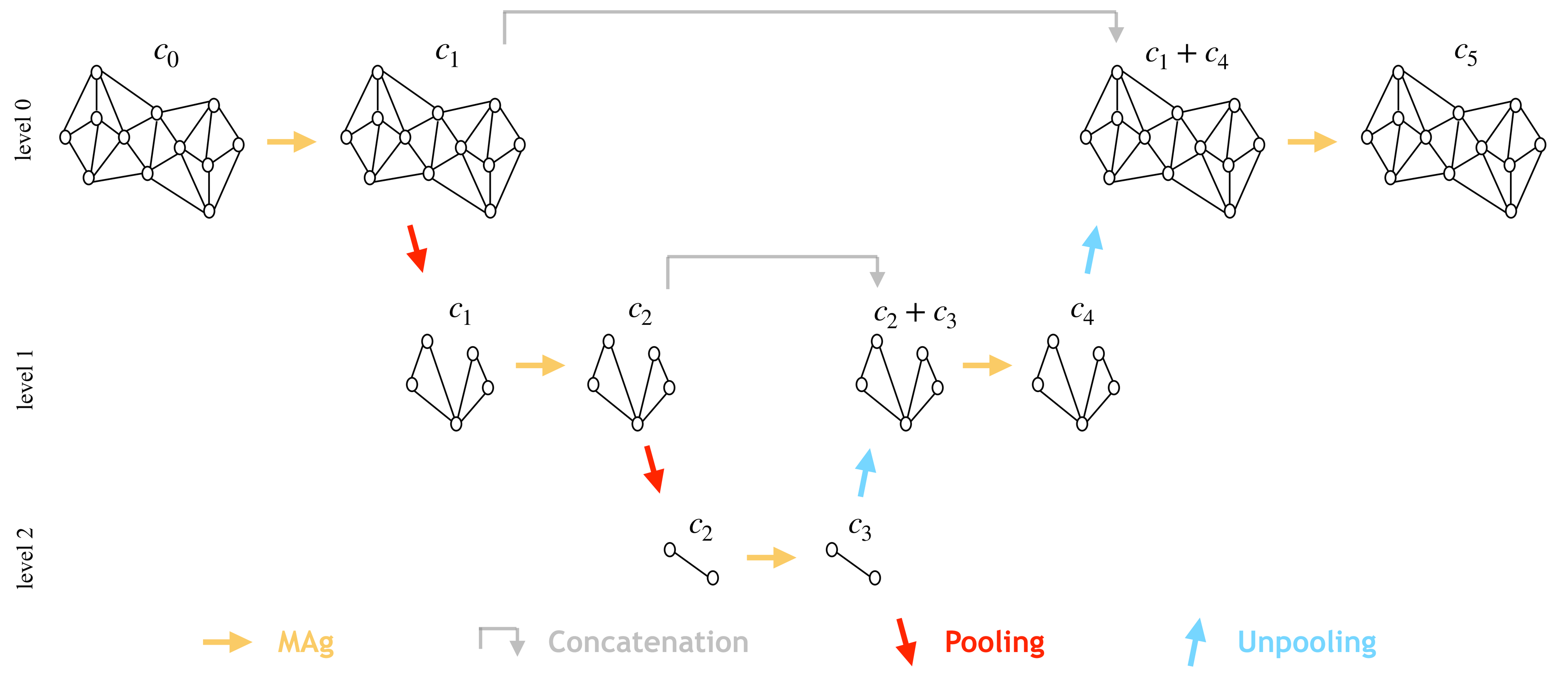


Figure 1. MAgNET: Multi-channel aggregation network [1].

Data Generation

Dataset $\mathcal{D} = (\mathbf{f}_i, \mathbf{u}_i)_{i=1}^{N}$, of pairs of nodal force, and displacement vectors is generated by applying random forces, using Neo-hookean hyperelastic law.

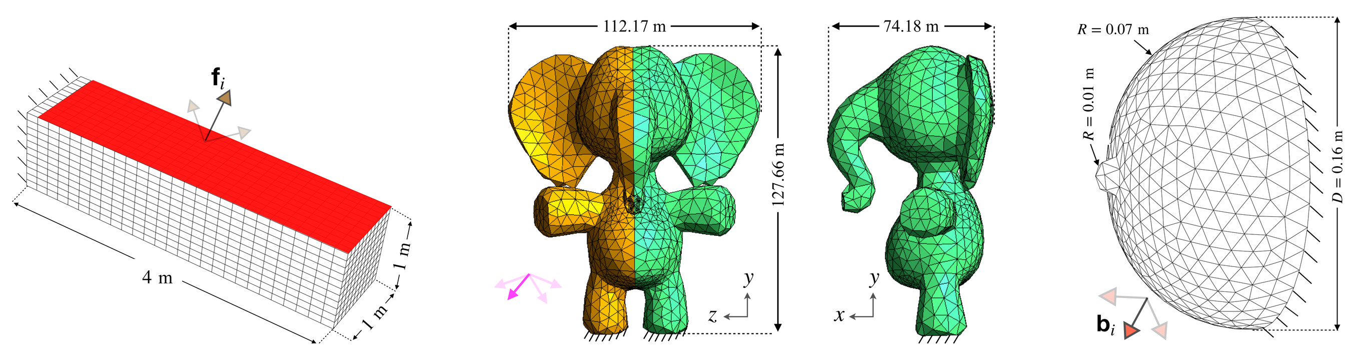


Figure 2. Schematics of three benchmark examples. Regions marked in red color indicate the nodes at which random nodal forces are applied to generate training datasets.

Training & Test Metrics

Training Loss: $\mathcal{L}_{\text{train}} = \frac{1}{N}\sum_{i=1}^{N} \|\mathcal{G}(\mathbf{f}_i) - \mathbf{u}_i\|_2^2$

Validation metric

For the test set $\{(\mathbf{f}_1, \mathbf{u}_1), ..., (\mathbf{f}_M, \mathbf{u}_M)\}$, $\mathcal{F}$=Degrees of freedom of mesh

$$e_m = \frac{1}{\mathcal{F}} \sum_{i=1}^{\mathcal{F}} |\mathcal{G}(\mathbf{f}_m)^i - \mathbf{u}_m^i|.$$

$$\bar{e} = \frac{1}{M}\sum_{m=1}^{M} e_m, \qquad \sigma(e) = \sqrt{\frac{1}{M-1}\sum_{m=1}^{M}(e_m - \bar{e})^2}$$

Results

Accuracy:

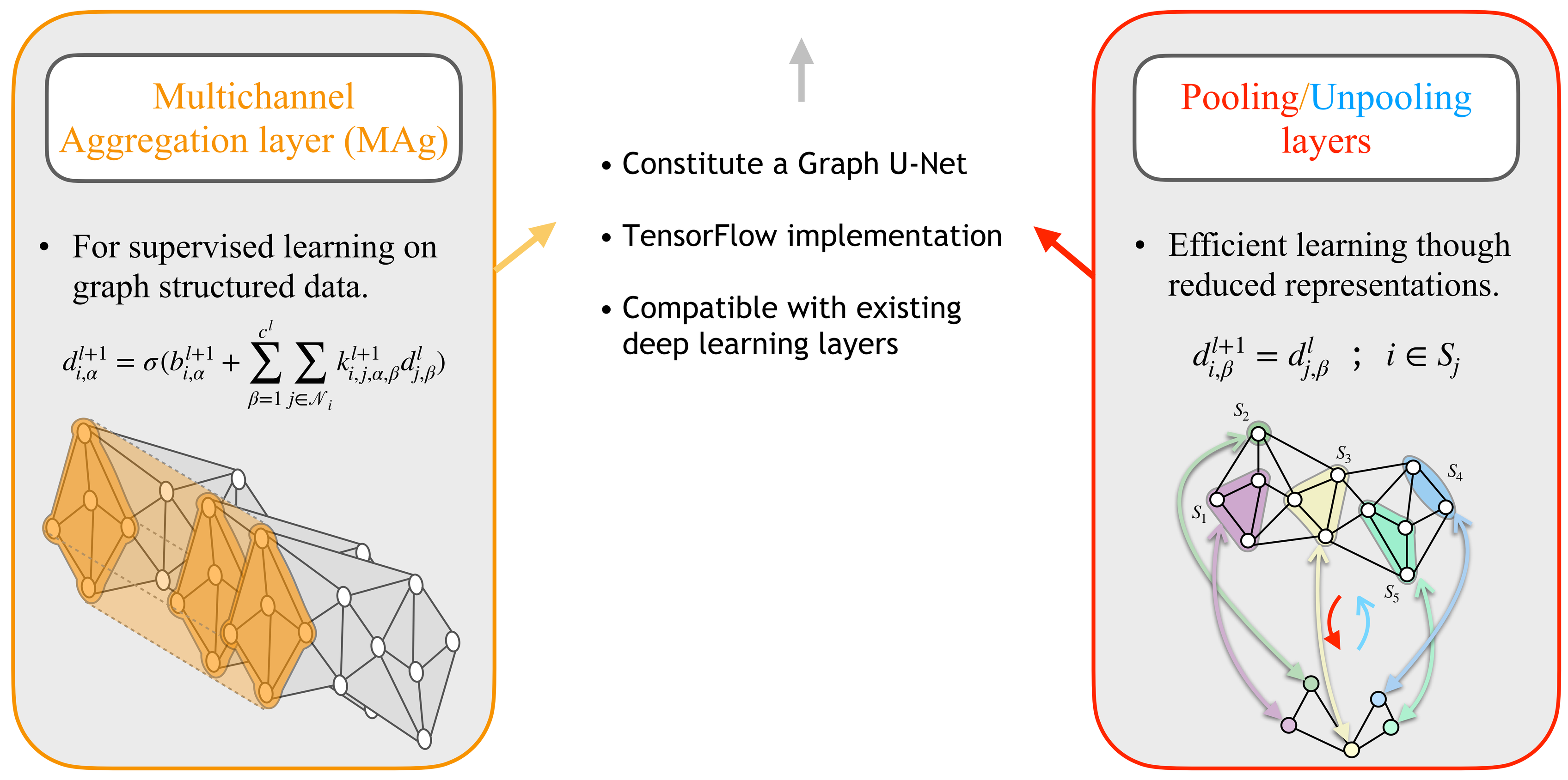
Example	$\mathcal{F}$	N	M	$\bar{e}$ [m]	$\sigma(e)$ [m]	Max disp [m]
Beam (MAgNET)	12096	33858	1782	0.8 E-3	0.7 E-3	1.47
Beam (CNN U-Net)				0.7 E-3	0.5 E-3	
Elephant (MAgNET)	5835	7600	400	8.9 E-3	1.9 E-3	140.01
3D breast (MAgNET)	3105			8.9 E-5	3.1 E-5	0.07

Table 1. Error metrics for the test sets.

Prediction times:

MAgNET offered **x40 speedup** in comparison to FEM simulations.

Proposed Deep Learning Layers



Visualisations

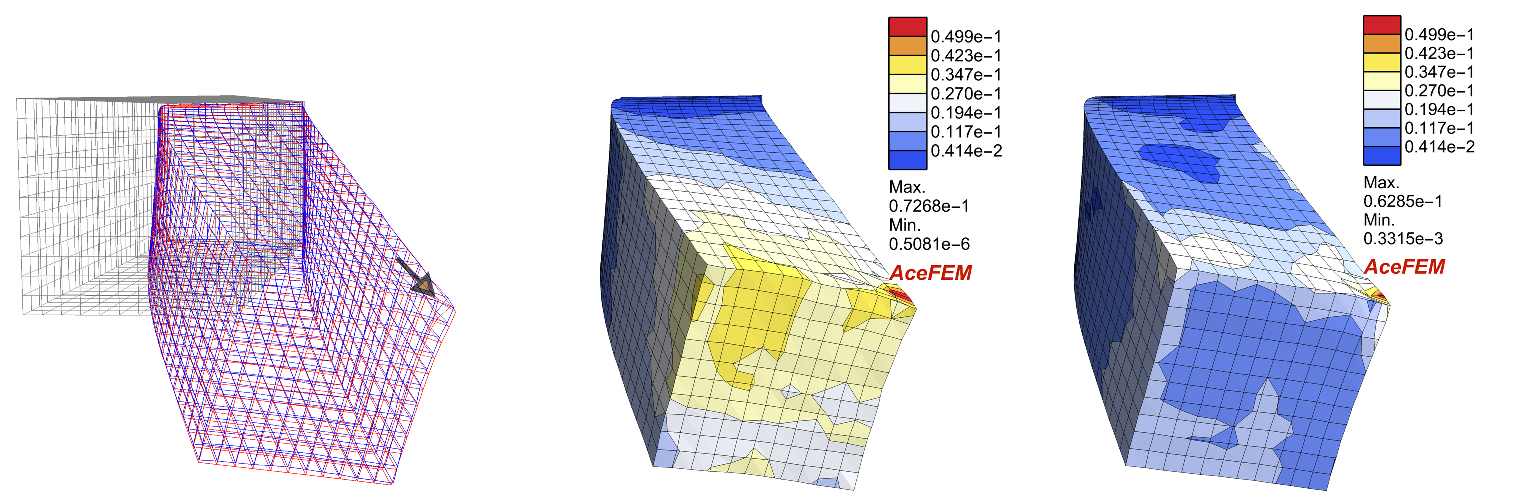


Figure 3. Deformation under point load. Error contours for MAgNET and CNN U-Net predictions, when compared to the FEM solution. The relative error for the prediction of displacement of node of application of load when compared to FEM is 4% for MAgNET and 3% for CNN U-Net.

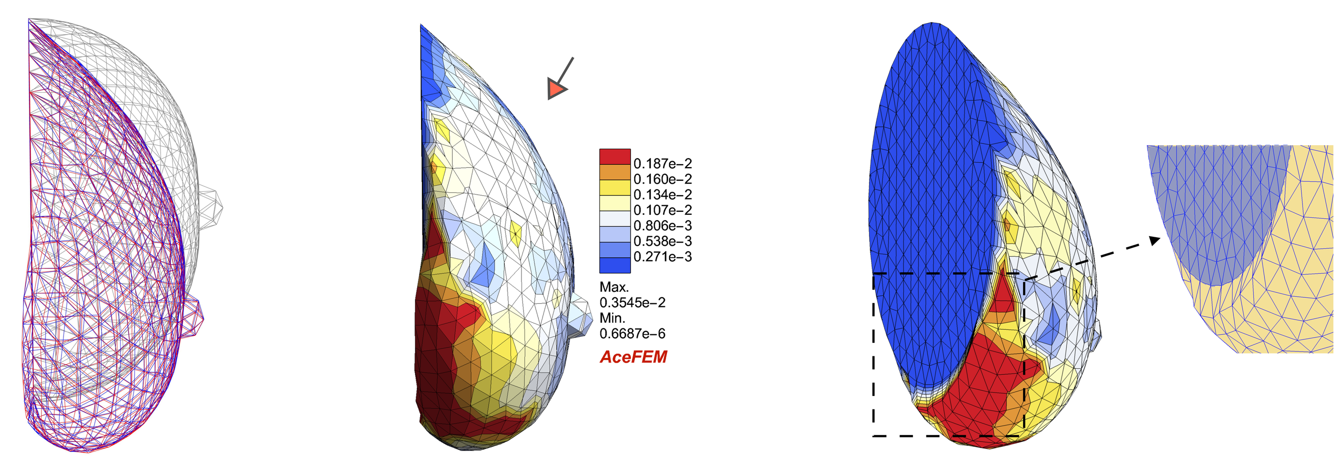


Figure 4. Deformation under body force computed using MAgNET. Maximum nodal displacement for this case is 0.07 m for the tip and relative prediction error for the same is 1%.

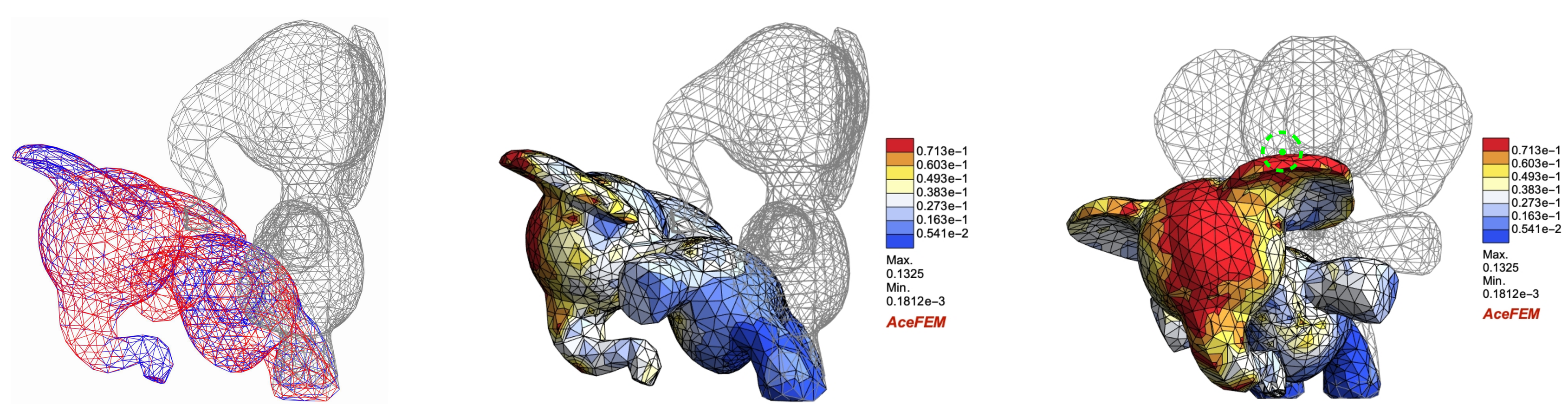


Figure 5. Deformation under body force computed using MAgNET. Maximum nodal displacement for this case is 140.01 m for the green node and relative prediction error for the same is 0.03%.

Conclusions

- MAgNET scales well and learns efficiently on arbitrary mesh inputs.
- MAg layer extended the concept of CNNs to non-grid inputs.
- MAgNET is an efficient surrogate model for non-linear FE simulations.

Reference

- S. Deshpande, S.P.A. Bordas, and J. Lengiewicz. *MAgNET: A Graph U-Net Architecture for Mesh-Based Simulations.* Arxiv 2023. DOI: https://doi.org/10.48550/arXiv.2211.00713.
- S. Deshpande, J. Lengiewicz, and S.P.A. Bordas. *Probabilistic Deep Learning for Real-Time Large Deformation Simulations.* Computer Methods in Applied Mechanics and Engineering, 2022. DOI: https://doi.org/10.1016/j.cma.2022.115307.
- S. Deshpande et al. *Convolution, aggregation and attention based deep neural networks for accelerating simulations in mechanics.* Frontiers in Materials, 2023. DOI: 10.3389/fmats.2023.1128954.

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