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

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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].

Data Generation

Dataset \(\mathcal{D} = (f_i, u_i)^N_{i=1}\) 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.](image)

Training & Test Metrics

Training Loss:
\[ \mathcal{L}_{\text{train}} = \frac{1}{N} \sum_{i=1}^{N} \| G(f_i) - u_i \|^2 \]

Validation metric
For the test set \(\{(f_1, u_2), ..., (f_M, u_M)\}, \mathcal{F}=\text{Degrees of freedom of mesh}, \)
\[ e = \frac{1}{M} \sum_{m=1}^{M} (u_m - \hat{u}_m) \]
\[ \sigma = \frac{1}{\sqrt{M-1} \sqrt{\sum_{m=1}^{M} (e_m - \bar{e})^2}} \]

Results

<table>
<thead>
<tr>
<th>Example</th>
<th>(\mathcal{F})</th>
<th>(N)</th>
<th>(M)</th>
<th>(e) [m]</th>
<th>(\sigma) [m]</th>
<th>Max disp [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beam (MagNET)</td>
<td>12096</td>
<td>33850</td>
<td>1782</td>
<td>0.8 E-3</td>
<td>0.7 E-3</td>
<td>1.47</td>
</tr>
<tr>
<td>Beam (CNN U-Net)</td>
<td>7.7 E-3</td>
<td>0.5 E-3</td>
<td>8.9 E-3</td>
<td>1.9 E-3</td>
<td>140.01</td>
<td></td>
</tr>
<tr>
<td>Elephant (MagNET)</td>
<td>5835</td>
<td>3.105</td>
<td>7600</td>
<td>400</td>
<td>8.9 E-5</td>
<td>3.1 E-3</td>
</tr>
</tbody>
</table>

![Table 1. Error metrics for the test sets.](image)

Prediction times:
MagNET offered \(x40\) speedup in comparison to FEM simulations.

![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.](image)

![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%.](image)

![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%.](image)

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


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