Real-Time Large Deformation Simulations Using Probabilistic Deep Learning Framework

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Motivation & Overview

Motivation

- Engineering applications, such as in the biomedical field demand accurate real-time non-linear deformation responses.
- Conventional techniques, such as FEM, are time-consuming.
- Deterministic models fail to account for uncertainties.
- Bayesian methods such as Gaussian processes, Markov chain Monte Carlo methods don't scale well with the problem size.

Solution

- Deep learning surrogate models to speed up the solutions.
- Bayesian inference to efficiently track uncertainties.

Implementation details

- U-Net ($\mathcal{U}$), a convolutional NN architecture is used.
- Deterministic and probabilistic models are proposed.
- U-Nets are trained on synthetic FEM datasets.
- Parameters of the network are Gaussian distributions.
- Variational Bayesian inference is implemented.
- **Prior means** are included in the **training procedure**.

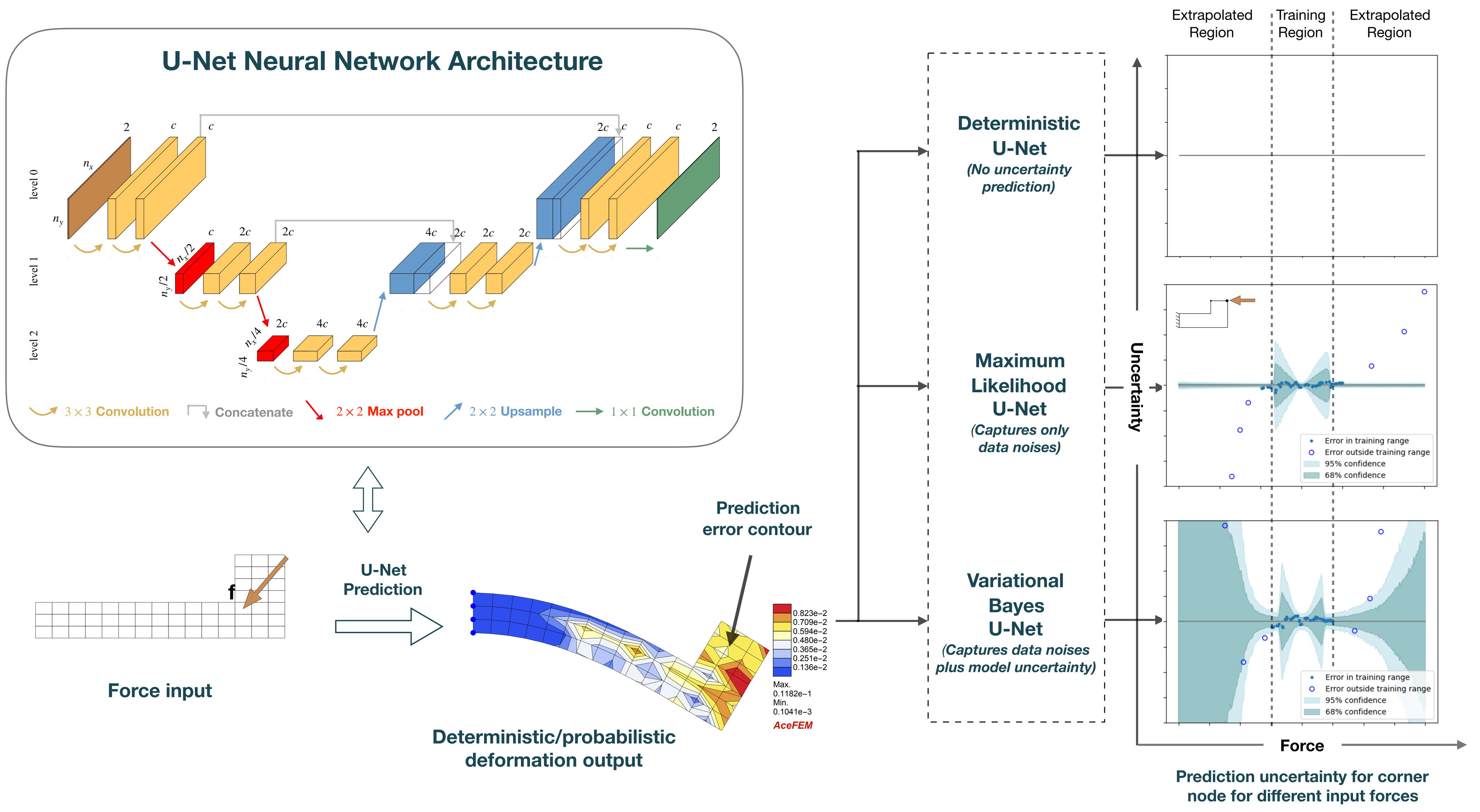

Figure 1. Overview of the framework [Deshpande et al. 2021].

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.

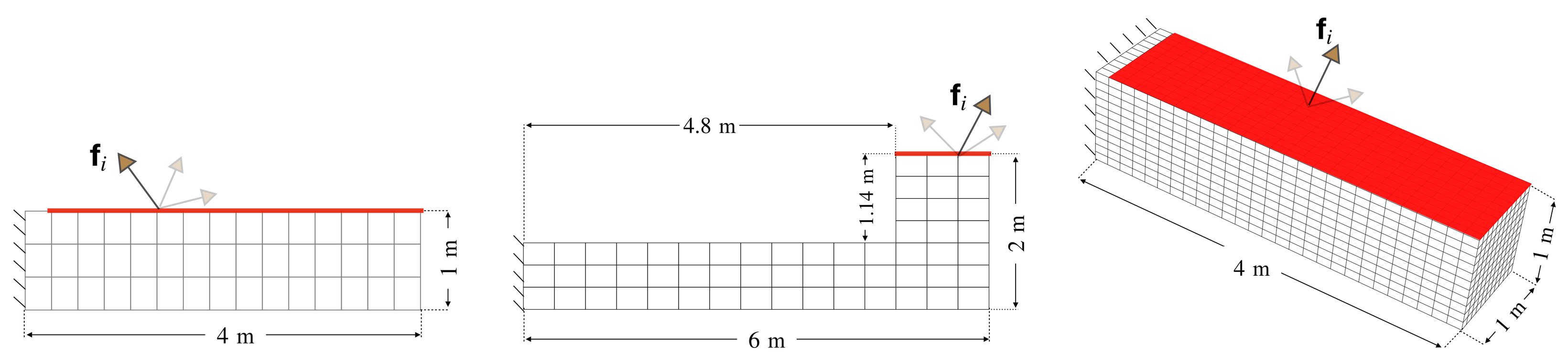

Figure 2. Schematics of three benchmark examples. Regions marked in red color indicate the nodes at which random nodal forces are applied to generate training datasets.

Training & Test metrics

Deterministic Loss: $\mathcal{L}_{\text{det}} = \frac{1}{N}\sum_{i=1}^{N} ||\mathcal{U}_{\text{Det}}(\mathbf{f}_i) - \mathbf{u}_i||_2^2$

Variational Bayes Loss: ($\mathcal{M}$ Monte Carlo samples used)

$$\mathcal{L}_{\text{VB}} = \text{KL}[q(\boldsymbol{w}|\boldsymbol{\theta})||P(\boldsymbol{w}|\mathcal{D})]$$
$$= \text{KL}[q(\boldsymbol{w}|\boldsymbol{\theta})||P(\boldsymbol{w})] - \mathbb{E}_{q(\boldsymbol{w}|\boldsymbol{\theta})}[\log P(\mathcal{D}|\boldsymbol{w})]$$
$$\approx \sum_{i=1}^{\mathcal{M}} \log q(\boldsymbol{w}^{(i)}|\boldsymbol{\theta}) - \log P(\boldsymbol{w}^{(i)}) - \log P(\mathcal{D}|\boldsymbol{w}^{(i)})$$

where

$q(\boldsymbol{w}|\boldsymbol{\theta})$ = Approximate posteriors for CNN parameters
$P(\boldsymbol{w})$ = Priors for CNN parameters
$P(\mathcal{D}|\boldsymbol{w})$ = Gaussian liklihood loss

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

$$e_m = \frac{1}{\mathcal{F}}\sum_{i=1}^{\mathcal{F}} |\mathcal{U}_{\text{Det/Bayes}}(\mathbf{f}_m)^i - \mathbf{u}_m^i|.$$

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

Reference

Deshpande, S., J. Lengiewicz, and S. P. A. Bordas (2021). *Probabilistic Deep Learning for Real-Time Large Deformation Simulations*. DOI: 10.48550/ARXIV.2111.01867. URL: https://arxiv.org/abs/2111.01867.

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Results

Accuracy:

Type	M	N	$\bar{e}$ [m]	$\sigma(e)$ [m]
2D Beam (VB)	300	5700	1.3 E-3	1.3 E-3
2D Beam (D)	300	5700	0.3 E-3	0.2 E-3
2D L-Shaped (VB)	200	3800	5.3 E-3	3.7 E-3
2D L-Shaped (D)	200	3800	0.8 E-3	0.4 E-3
3D Beam (D)	1782	33858	0.6 E-3	0.3 E-3

Table 1. Error metrics for test sets. M= No. of test examples, N=Number of training examples D = Deterministic, VB = Variational Bayes.

Prediction times:

Type	dof	$\text{t\_fem}_{\text{CPU}}$ [s]	t_{CPU} [s]	t_{GPU} [s]	$\frac{\text{t\_fem}_{\text{CPU}}}{t_{\text{CPU}}}$	$\frac{\text{t\_fem}_{\text{CPU}}}{t_{\text{GPU}}}$
2D Beam	128	0.123	0.005	0.001	25	123
2D L-shaped	256	0.120	0.007	0.001	17	120
3D Beam	12096	3.1	0.1	0.009	31	**345**

Table 2. Prediction times of deterministic U-Net on CPU & GPU.

Visualisations

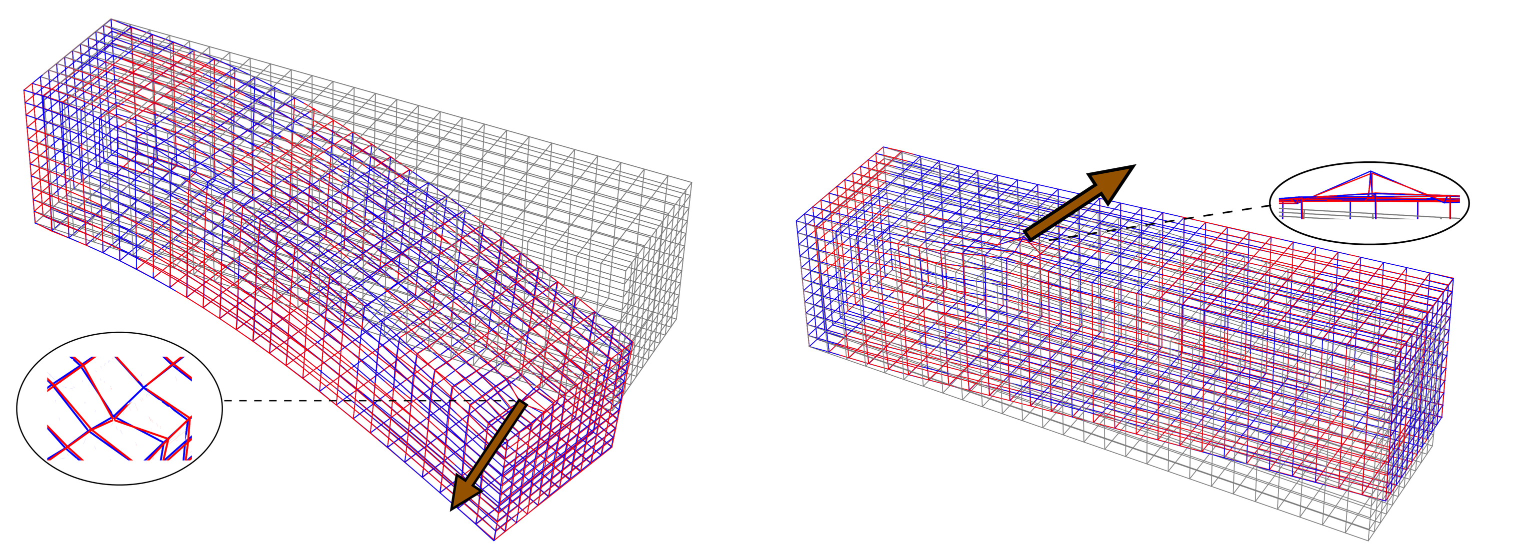

Figure 3. Deformation of 3D beam computed using deterministic U-Net (blue), reference FEM solution (red) is present. The magnitude of tip displacement for the first case is 1.1 m (0.6% error) and for the second case is 0.26 m (1.6% error).

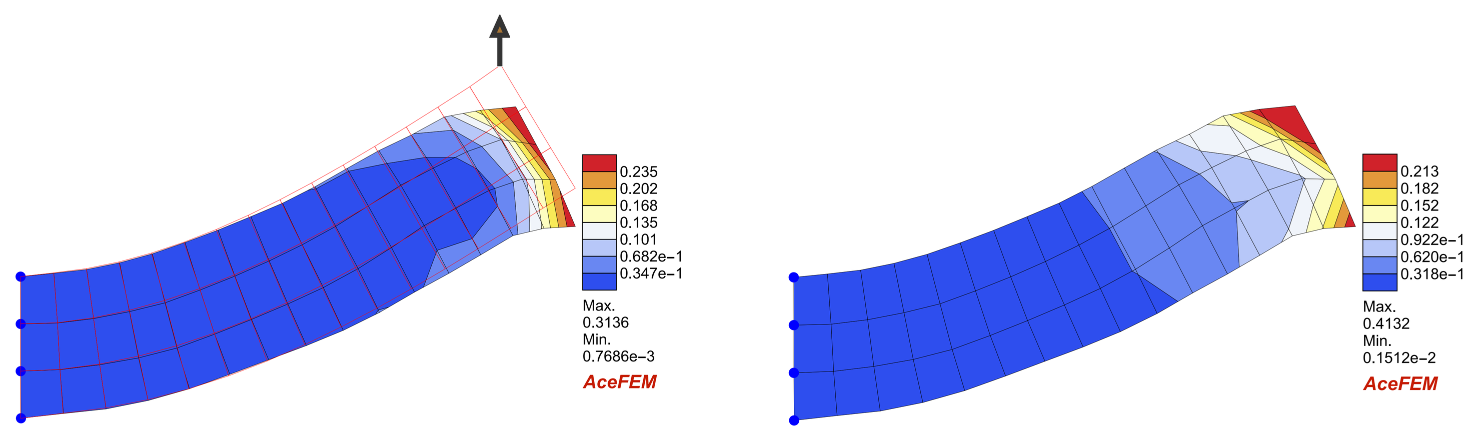

Figure 4. Deformation of 2D Beam using Bayesian U-Net for an input force outside the training range. Strong co-relation of error (left) and uncertainty predicted using Bayesian U-Net (right).

Conclusions

- Accurate large deformation solutions **computed in milliseconds**.
- Data noises and neural network model **uncertainties are captured**.
- Qualitative agreement between model errors and computed uncertainties.
- Captured the effect of increased uncertainty in the regions not supported by data.

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