Data Preprocessing

The FEM model data (.vtk file) contains points and cells information but can not be directly used for ML models. The strain information is stored in cells and, normally, the number of points is greater than the number of cells; however, in this case, the number of points is much less, which created difficulty for transforming data from mesh to high dimensional array. The current data preprocessing can be summarized as follow

1. Exporting cell center coordinates and their corresponding strain values using ParaView.
2. Creating 3-dimensional arrays for storing the strain values based on the coordinates. The original size for strain in each direction after transforming is (891,897,465).
3. Interpolating the array to match the microstructure dimension using `scipy.ndimage.zoom` to generate 6 3-dimensional arrays (since for each cell, there are 6 strain values). The size of the array after interpolation is (300,300,152)
4. Combining 6 strain arrays and microstructure array into one of which the shape is (7,300,300,152).
5. For training purpose, randomly sampling 2000 data points with window size of (16,16,16) from the array in the previous step.

Deep learning models

The deep learning models are based on the work from the paper (https://arxiv.org/pdf/1808.08914.pdf) that worked on stress field prediction for two-dimensional images (microstructure, loads, etc) by convolutional neural network based models. Some changes have been made to fit our data, but the network architectures are the same, which are shown in fig 1 & 2.

The implementation of both models are done in `Tensorflow`. The data were split into training set to train the networks and validation set to evaluate models with a ratio of 8:2. The training and validation results after 1000 epochs can be found in table 1.

	Training R^2	Validation R^2
SCS	0.8894	0.2661
StressNet	0.9633	0.3539

Table 1: Training and validation coefficient of determination of SCS and StressNet models. The validation R^2 are the highest value they reached with in 1000 epochs of training.

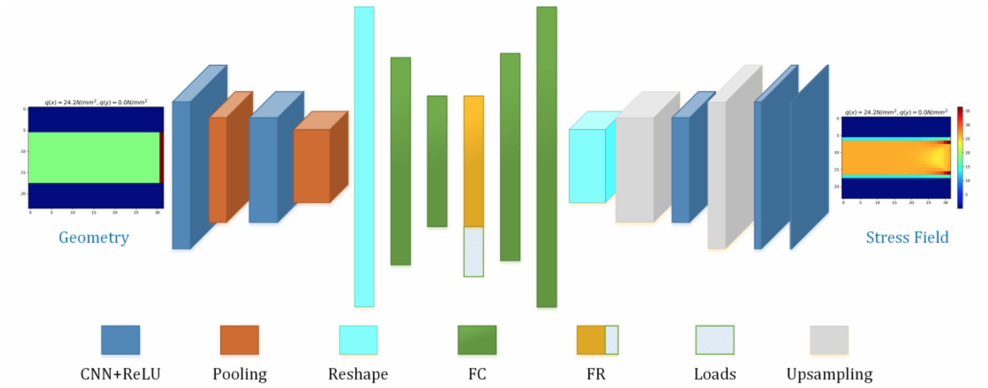

Figure 1: The single channel input network [1], consisting of basic convolutional operations with a encoder-decoder structure. Input is the 3-dimensinal microstructure and the output is the corresponding strain field which is represented in a 4 dimensional array for each data point.

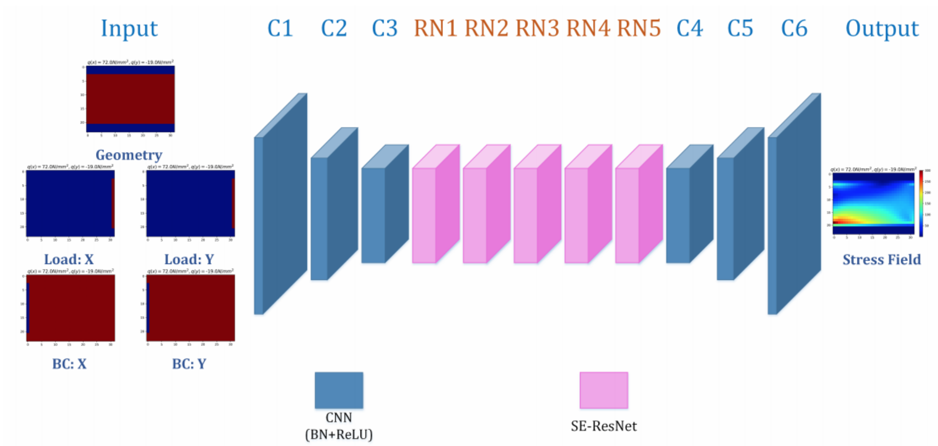

Figure 2: StressNet [1], the main contribution of the aforementioned paper. It incorporates residual blocks, which are able to model identify mapping, and SE blocks, which can adaptively recalibrates channel-wise feature responses. Due to the fact that the only available input is the microstructure, the number of channels for the input is just 1.

The results indicate a poor generalization ability of both models, where StressNet has better performance on fitting training data than the baseline SCS network due to its higher complexity. The models seem to only "remember" what is in the training set instead of "learning" enough of the underlying mapping from the microstructure to its strain field. These results are within our expectation, since we only have microstructure as input which can be considered a 3-dimensional array with only 1 channel, but the channels of the output increases to 6.

More information might be needed, such as boundary conditions and loads. In addition, the small data size could limit the models to learn. The next attempt would be using 3D-GAN [2] to generate more data that are similar to the current data, and use them for the models to learn better.

References

[1] Z. Nie, H. Jiang, and L. B. Kara, "Stress field prediction in cantilevered structures using convolutional neural networks," *Journal of Computing and Information Science in Engineering*, pp. 1–11, 2019.

[2] J. Wu, C. Zhang, T. Xue, B. Freeman, and J. Tenenbaum, "Learning a probabilistic latent space of object shapes via 3d generative-adversarial modeling," in *Advances in neural information processing systems*, pp. 82–90, 2016.