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A 3D Bayesian Multiscale Graph Neural Network Framework To Predict Local Stress Fields In Structures With Microscale Features

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Multi-scale structures are very common in mechanical and bio-mechanical applications, for instance composite and porous materials. Full Finite Element Analysis (FEA) for stress prediction is usually very expensive in these structures as the FE mesh needs to be very dense to capture the effect of the fine scale features.

Common approaches to tackle multiscale problems usually fall either in the homogenisation or domain decomposition techniques. In both cases the multiscale problem is split into a macroscale and a microscale problem. In homogenisation the microscale computations are performed over a representative volume element (RVE), assuming that the macroscale displacement gradients do not vary over the material sample. If that is not the case, domain decomposition methods are employed where the results of homogenisation are applied to the boundary of regions of interest for concurrent microscale corrections to be performed [4]

In this work we propose a Neural Network (NN) based domain decomposition method to tackle 3D multiscale problems. A wide range of NNs have recently been used to learn the response of FE models in computational mechanics problems. NNs with fully connected layers have been used for instance in [1] but most commonly Convolutional Neural Networks (CNNs) are employed that are very efficient in working with images [6]. Unfortunately, the computational cost involved in training a CNN for 3D multiscale problems where the resolutions has to be very fine to reflect the effect of the microscale features is prohibitive.

To overcome this problem, we choose to train a Graph NN (GNN) that can operate directly on the FE mesh used to create the training data. In contrast to images that have a fixed resolution the FE mesh can be much denser in areas where the geometry is complicated or we expect big gradients of our quantity of interest and much coarser everywhere else [3]. We use the formulation from [2] that allows for a very natural encoding of information on the mesh where absolute information can be encoded on the vertices of the mesh while relative information is encoded on the edges of the mesh.

Lastly, we opt for a Bayesian GNN that is able to quantify the uncertainty of the prediction and provide not only a mean estimation but also credible intervals for the prediction. We use the MC dropout method [5] to keep the computational cost at minimum.

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