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Predicting High-Stress Regions Inside Microstructure Using Deep Learning

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A deep learning-based Encoder-Decoder model to predict the characteristics of high-stress clusters (stress-hotspots) inside a given microstructure under an applied load was developed. Further, we analyze the trained model to understand the microstructure features causing these stress hotspots. A microstructure is a small-scale structure observed at the microscale. It is composed of multiple grains, where each grain represents an arrangement of atomic crystals in a particular orientation. The microstructure amplifies the applied load creating hotspots, causing nonlinear phenomena such as fracture and yielding. However, there is no known analytical/ statistical relationship between microstructure features and hotspots characteristics.

Numerical schemes such as finite element and Fourier-based methods can obtain highly accurate stress fields in microstructure samples. However, simulating a large number of samples and then manually observing the relationship between hotspots and the microstructure features is complicated and can suffer from user bias. Statistical models can help to infer such relationships using the data generated from these numerical schemes. However, the microstructure samples and the stress obtained from simulation are high-dimensional images. Moreover, there exist local-spatial relations between microstructure images and stress images. The proposed Encoder-Decoder model, based on convolutional filters, can capture local-spatial relations in high-dimensional images using spatially weighted averaging operations.

The model was trained against linear elastic calculations of stress under an applied load in a synthetically generated microstructure. The model prediction accuracy was analyzed using the cosine similarity metric and by comparing the peak stress clusters' geometric characteristics against the ground truth. The average cosine similarity on the test set is around 0.95, which is very close to 1.0 (perfect prediction). The model can predict the location and size of the stress hotspots and perform better for hotspots around higher values of the peak stress. Further, to understand the relationship between microstructure features and hotspot characteristics using the trained model, we use feature visualization and gradient visualization methods. In our preliminary analysis using feature visualization methods, it was observed that different convolutional filters in the first layer capture different but distinguishable local features such as grains and grain boundaries in a microstructure. The behavior of these filters around hotspots can be used to understand the relation between hotspots and microstructure features. Using gradient visualization methods, we have observed some long-range interaction inside a microstructure.