

ABSTRACT

How to Predict Material Behavior by Utilizing Neural Networks

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The numerical simulation of materials poses significant challenges and requires considerable computational resources, especially when dealing with complex microstructures, multiscale phenomena, and damage evolution. Neural networks offer a promising way to alleviate this computational burden by reducing the costs associated with solving the highly nonlinear and time-dependent partial differential equations (PDEs) that characterize such systems [1,2]. Here, a spatio-temporal surrogate model was developed, which is capable of predicting crack initiation and propagation in complex heterogeneous material microstructures, as well as generating the full stress-strain response using concrete microstructures as an example.

To achieve this, the developed surrogate model uses the U-Net architecture with a novel adaptation in combination with a convolutional neural network. Instead of relying on pixel data, the input to the U-Net consists of spatial distributions of four different material properties, namely the Young's modulus, fracture energy, ultimate tensile strength, and the spatial distribution of the damage index at a certain step frame. Based on this input data, the U-Net model is able to predict the spatial distribution of the damage index for the subsequent time step. Based on this information, the downstream convolutional neural network computes the resulting homogenized stress value. It is shown that this approach achieves high prediction accuracy with a training dataset of just 500 samples and effectively captures the complex physics of fracture mechanisms in concrete microstructures.

[1] A. Gupta, A. Bhaduri and L. Graham-Brady, *Mech. Mater.*, 184, 104709 (2023).

[2] S. Li and S. Hou, *Int. J. Mech. Sci.*, 266, 108952 (2024).