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Neural network surrogates for stress field prediction in heterogeneous materials

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Abstract

Solid materials are often considered homogeneous at the macroscopic scale. However, finer-scale features can influence their macroscopic behavior. Many materials, including composites and polycrystals, are inherently heterogeneous at the micro- or mesoscopic scale. Therefore, taking into account these different scales in numerical models can help improve the design of mechanical parts and structures. Multiscale models usually use homogenization and/or localization to bridge these scales. This requires computing stress and strain fields in representative volume elements (RVEs), which explicitly model the material heterogeneity. However, these computations are often expensive, which limits the adoption of multiscale models in engineering applications. Recent studies have proposed using neural networks to accelerate the computation of stress and strain fields in RVEs. The input is generally the microstructure and the macroscopic loading, and the output is the microscopic stress or strain fields. The training data is typically generated by traditional numerical solvers. Once training is completed, the neural network can be used to predict an approximation of microscopic fields for unseen microstructures and loading conditions, as long as they are not too different from the training data. This approach has shown significant acceleration of multiscale simulations across a range of microstructure morphologies and material behavior. In this work, we study the computational aspects of this approach when scaling to high-resolution 3D RVEs and the generalization capability of convolutional neural networks (CNNs). We generated concrete mesostructures with different aggregate shapes and volume fractions. Mesoscopic stress and strain fields were precomputed using an FFT-based solver with multiple stiffness ratios between aggregates and the cementitious matrix. The mesostructures are periodic and discretized in voxels using 64^3, 128^3, and 256^3 resolutions. The hyperparameters of the neural network architecture are automatically optimized using Bayesian methods for different objectives: maximizing accuracy, and achieving a user-specified balance between accuracy and inference speed. We also investigated data augmentation and generalization capability across datasets with varying mesostructure morphologies and material properties. The computational cost of data generation, training, and inference on different hardware (laptop and cluster CPUs and GPUs) is analyzed. We believe this work contributes to the understanding of surrogate modeling in multiscale simulations and introduces a general framework for selecting optimal architectures based on user requirements for accuracy and computational efficiency. Code and data will be made publicly available.

Keywords:

neural network heterogeneous materials stress field concrete mesostructure