Uncertainty Quantification in Multiscale Modeling of Composite Materials Using Physically Recurrent Neural Networks

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Multiscale modeling of composite materials accurately predicts material behavior but faces high computational costs. To address this issue, neural networks have been used as surrogates for full-order micromodels, predicting their complex behavior accurately. Physically Recurrent Neural Networks (PRNNs) [1] recently demonstrated excellent accuracy for microscale and multiscale simulations with fixed material properties, significantly reducing computational time and requiring minimal training data compared to conventional recurrent neural networks (RNNs). Unlike conventional RNNs, where parameter changes typically require extensive retraining or feature expansion, PRNNs embeds material models in their material layer, which enables modifying material parameters after training.

This study investigates whether a PRNN pretrained on a fixed set of material parameters can maintain accuracy for varying material properties, and thus propagate uncertainty of these properties in a multiscale framework. When material properties are kept fixed during testing, mimicking the rigidity of a conventional RNN, the network loses its accuracy. However, when material properties are adjusted during testing according to the input, PRNN shows high accuracy across a wide range of parameters, accounting for variations in material properties without having to retrain the network.

To evaluate the effect of microscale parameter variations on macroscale responses, multiscale uncertainty quantification (UQ) is performed by comparing full-order and PRNN-driven simulations on an overly coarse mesh. PRNN reduces simulation time by over 7000 times while accurately capturing highly nonlinear force distributions. A PRNN-driven UQ is demonstrated on a more accurate finer mesh, where a full-order UQ would require decades to compute. These results show that otherwise too costly UQ in multiscale modeling of composites becomes possible using PRNNs as an accurate surrogate for full-order micromodels.

References
[1]   M.A. Maia, I.B.C.M. Rocha, P. Kerfriden, F.P. van der Meer, (2023). Physically recurrent neural networks for path-dependent heterogeneous materials: Embedding constitutive models in a data-driven surrogate, *Computer Methods in Applied Mechanics and Engineering* 407, 115934.

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