Goal-oriented reduced order model adaptivity assisted by artificial neural networks

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ABSTRACT

Multi-scale simulation of complex heterogeneous microstructured materials is a challenging task in materials research and industrial design. The efficiency of traditional finite element (FE) simulations reaches quickly its limits on the macroscale due to the complexity of heterogeneous materials with rich microstructure. The lack of simulation efficiency, specially for many query problems, stimulated the research of physically motivated reduced order models and purely data-driven surrogate models. Highly efficient reduced order models with physical motivation have been published in literature. More recently, purely data-driven approaches have gained incredible momentum due to new achievements in computational power, kernel methods and machine learning approaches, see, e.g., [1] and [2].

The present contribution aims at the combination of a reduced order model (ROM) and artificial neural networks (ANN) in goal-oriented problems with certain quantities of interest. From high-fidelity mechanical microstructure FE simulations with effective strains as input data, a large reduced basis is identified in order to build the ROM. Trivial lower dimensional sub-bases of the large reduced basis are selected for less expensive computations and comparison of accuracy. The quantity of interest for the microstructure simulations at hand is the effective stress, which is regarded as the output data. Based on the FE data and on the ROM, ANNs are trained to calibrate (1) an effective stress surrogate based on the FE effective stress and (2) error surrogates for the quantity of interest for the reduced basis and its sub-bases. Different strategies for the calibration of error estimates are presented for pure regression and classification approaches. Hereby, error estimates can be calibrated to deliver rather conservative results in order to ensure safety in respect to failure. This is achieved by designing the objective / loss function for the training of the respective ANNs. The calibrated ANNs are then used to first predict an effective stress for a given effective strain and check its predicted error. If the predicted error is too large, then the ROM error surrogates are used to adaptively scan for a minimum ROM dimension according to the prescribed tolerances. This offers an adaptive scheme, which takes advantage of modern highly efficient and computationally inexpensive evaluations of trained ANN, while computationally more expensive but highly accurate ROMs are only used if the ANN is not able to achieve certain tolerances. Results for the consideration of the ROM residual as an additional input in the ANNs are presented. As an example, a physically nonlinear pseudo-plasticity model for a three-phase composite is taken into account and the results of the presented strategies are discussed.

REFERENCES

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