Deep Material Networks

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Abstract

In multiscale simulations traditional data driven methods have failed to produce reliable results for highly nonlinear problems in comparison to classical numerical computational homogenization algorithms. Deep material network is a novel hybrid machine learning solver framework which gives reliable predictions in the nonlinear elastic domain with just training using linear elastic responses. The work discusses the implementation of this workflow and successful benchmarking of this technology for state-of-the-art case studies.

1 Introduction

There are many areas of industry, where detailed material characterization is required. For examples, to deal with complexities of modern manufacturing processes like injection molding or even geological exploration in oil and gas industry namely digital rock physics et al [2013]. In all these applications, experimental material characterization is complemented with virtual multiscale simulation models which are calibrated by the earlier. Availability of modern micro computed tomography (μ-CT) imaging helps to capture detailed microstructure topologies. State-of-the-art algorithms like FFT based homogenization algorithms, first proposed by Moulinec and Suquet [1994], have enabled to solve the Lippmann-Schwinger equation in elasticity directly on the material images without need for meshing. However due to high resolution of μ-CT images, running direct numerical schemes like FFT homogenization becomes very slow especially for highly nonlinear material behaviours. Recent emergence of machine learning methods approximates the micro problem using artificial neural networks. Such methods suffer from low reliability of prediction away from the training set and also lack of thermodynamic consistency Fritzen et al. [2019]. To ensure reliability of the prediction, there is a need to build machine learning models that have mechanistic understanding of the physics.

2 Design

Liu et al. [2019] proposed the Deep Material Networks(DMN) framework which fits the linear elastic mechanical response of complex microstructure to hierarchical laminates. These laminates are then equipped with the same material models and boundary conditions as the complex microstructure to get equivalent response in the nonlinear elastic space. Figure 1 illustrates the basic paradhym of these hybrid models with mechanistic building blocks. Further Gajek et al. [2020], proposed a simpler, faster DMN which is thermodynamically consistent. The direct DMN approach introduced by Gajek et al. [2021], which proposes a vectorization of the online variational problem as a newton solution scheme with sparsification, was implemented in this work. Figure 2 shows the basic workflow in achieving an inelastic response from just linear elastic training.

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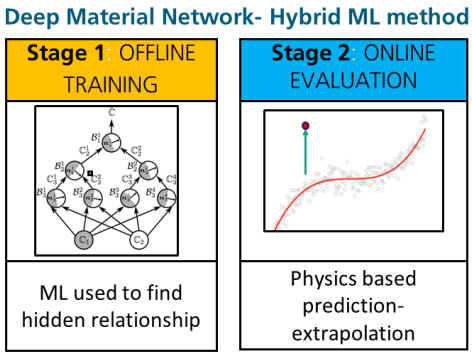

Figure 1: Basic theme of DMN.

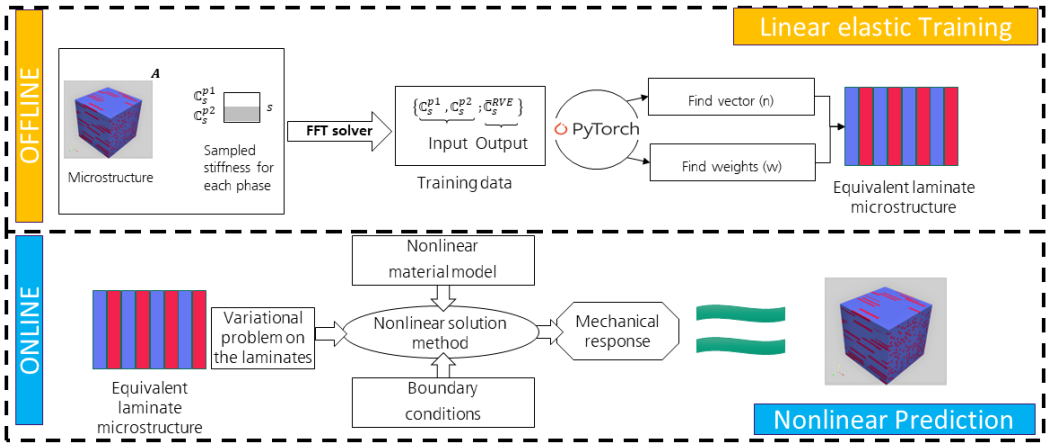

Figure 2: The basic workflow of a direct Deep Material Networks.

3 Evaluation

In order to evaluate the correctness of the implemented DMN, viscoelastic sampling was done similar to the implementation of Gajek et al. [2023]. After hyperparameter tuning in the offline training, the resulting DMN was used to perform inelastic experiments. The results of the experiments was campared against full field FFT direct numerical simulations and the speeds for viscoelasticity was benchmarked along with accuracies.

Table 1: Accuracies and speed up factor for viscoelasticity

Runtime comparison		
Name	Runtime	Number of threads
DMN runtime	<100 seconds	1
Full field FFT	51 hours	24
Speed up and errors		
Name	Value	
Speed up factor	44064	
Inelastic error	<2%	

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