A hybrid approach for the multi-scale simulation of irreversible material behavior incorporating neural networks

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The present contribution presents a hybrid approach for the multi-scale modeling where the yield surface and evolution equations are represented by neural networks, for which micro-scale simulations are used as training data. The approach and its implementation into a commercial finite element code are demonstrated for a ductile foam material. The results are verified by comparison with an FE simulation.

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1 Introduction

The mechanical behavior of materials is greatly influenced by their micro-structure. The irreversible processes at the micro-scale and their effect on the macroscopic behavior can be simulated within the computational homogenization framework. However, such multi-scale simulations within the FE framework are very expensive. In contrast, phenomenological constitutive equations at the macro-scale are often not flexible enough to reproduce the complexity of irreversible mechanisms and their interactions.

The representation of constitutive relations by machine learning approaches like neural networks has been proposed as a third way of material modeling. A review of application of machine learning methods in material science can be found in [1]. For constitutive modeling, the main challenge is to choose the response functions to be represented by neural networks. Some authors represented a non-linear stress strain relation, e.g. [2], corresponding to an inherent Cauchy elastic relation, whereas others represented the strain-energy density, corresponding to a hyper-elastic material, e.g. [3]. Very few attempts have been presented to represent irreversible material behavior. A recurrent neural network has been employed in [4] to model the irreversible behavior, requiring, however, cyclic and relaxation tests even for the uniaxial case.

2 Hybrid Multi-Scale Neural Network Approach (HyMNNA)

In the present approach, qualitative features of the expected macroscopic material behavior are already incorporated in the constitutive framework. In contrast to conventional phenomenological modeling, the open constitutive functions are not parametrized by a finite number of constitutive parameters, but are represented by neural networks.

Considered is for example here a foam made of elastic-plastic bulk material as shown at left-hand side of Fig. 1. From the fact that the bulk has a linear-elastic domain, it can be concluded that the foam has this property as well and the constitutive relation of the foam is thus formulated in a small deformation framework as

\[
\Sigma_{ij} = \bar{C}_{ijkl} E_{kl} = \bar{C}_{ijkl} \left( E_{kl} - E_{kl}^{pl} \right)
\]  

Fig. 1: Hybrid Multi-Scale Neural Network Approach (HyMNNA) [5]

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Furthermore, the bulk material exhibits rate independent behavior. This behavior is thus expected at the macroscale and can be described by a yield condition

\[
\Phi = \| \Sigma_{ij} \| - NN^\Phi \left( I_1, E_{pl}^{eq}, E_{pl} \right) \leq 0
\]  

Therein, \( NN^\Phi \) represents a neural network which represents the dependency of the yield function on the first stress invariant \( I_1 \) as well as the hardening via the dependency on the accumulated plastic strain \( E_{pl}^{eq} \). The dependency on \( E_{pl}^{eq} \) accounts for the cubic anisotropy of the micro-structure. The neural network is trained \textit{offline} from RVE simulations, which are performed for certain levels of multiaxiality. The actual macroscopic FEM simulation requires then the relatively cheap \textit{online} computation of the neural network response function within the material routine, Fig. 1. The latter has been implemented into the commercial FE code Abaqus/Standard via the UMAT interface. Further details on the approach, flow rule, extraction of training data from the RVE simulations and implementation can be found in [5, 6].

3 Example

The deformation of a thick foam specimen under bending-type loading due to a lateral pressure is considered as shown at right-hand side of Fig. 1. Details on the employed material parameters, dimensions and material parameters can be found in [5] as well.

![Fig. 2: Computed stresses in comparison to FE\(^2\) simulation](image)

Figure 2 shows the stresses computed with the HyMNNA approach in comparison to a corresponding \( FE^2 \) simulation. The latter represents the maximum level of accuracy that can be gained with homogenization approaches as used for the training in HyMNNA. The comparison of both approaches in Fig. 2 indicates a very good qualitative and quantitative agreement, even at the support, where the strongest plastic deformations occur. However, the HyMMNA approach provides an acceleration by a factor of 142, even though the \( FE^2 \) simulation has already been performed by a highly efficient monolithic scheme [7] (The latter taking 1h 36’42” on an Intel\textsuperscript{\textregistered} Xeon\textsuperscript{\textregistered} CPU X7542 using 16 cores).

4 Summary

The Hybrid Multi-Scale Neural Network Approach (HyMNNA) allows highly efficient macroscopic simulations based on a number of RVE simulations as training data. The results have been verified by comparison to an \( FE^2 \) simulation.

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