Received: 15 June 2021 | Accepted: 23 September 2021

DOI: 10.1002/pamm.202100069

Efficient two-scale simulations of microstructured materials using deep material networks

Sebastian Gajek[1,*], **Matti Schneider**[1], and **Thomas Böhlke**[1]

[1] Karlsruhe Institute of Technology (KIT), Institute of Engineering Mechanics (ITM)

Deep material networks (DMN) are a promising piece of technology for accelerating concurrent multiscale simulations. DMNs are identified by linear elastic pre-computations on representative volume elements, and serve as high-fidelity surrogates for full-field simulations on microstructures with inelastic constituents. The offline training phase is independent of the online evaluation, such that a pre-trained DMN may be applied for varying material behavior of the constituents. In this contribution, we investigate a two-scale component simulation of industrial complexity accelerated by DMNs. To this end, a DMN is solved implicitly at every Gauss point to include the microstructure information into the macro simulation.

1 Introduction

Many common engineering materials used for industrial applications, e.g., fiber reinforced composites or polycrystals, feature a spatially varying, complex microstructure. To harness the full potential of such materials, the microstructure information needs to be accounted for in mechanical simulations on the component scale. For this purpose, concurrent multiscale methods couple simulations on the micro- and macroscale. However, these approaches come with considerable computational costs which quickly become prohibitive for increasingly complex components.

As a remedy, a variety of approaches, ranging from model-order reduction techniques to machine learning approaches, were developed focusing on speeding up the micro simulation. In this work, we focus on so called deep material networks [1–3], a specific data-driven approach. A DMN serves as a surrogate model for full-field simulations on the microscopic scale. DMNs can be used in concurrent multiscale simulations giving rise to the so called FE-DMN [4] method.

2 Direct deep material networks

A two-phase direct DMN consists of a perfect, ordered binary tree of depth K, where every node of the tree is represented by a two-phase laminate, see Fig. 1(a) for a schematic. The DMN topology is uniquely determined by the laminates' directions of lamination $\vec{\boldsymbol{n}} = \left[\boldsymbol{n}_1^1, \boldsymbol{n}_2^1, \boldsymbol{n}_2^2, \dots\right]$ and the weights $\vec{\boldsymbol{w}} = \left[w_{K+1}^1, w_{K+1}^2, \dots\right]$, which represent a re-parameterization of the laminates' volume fractions.

To identify the free parameters $\vec{\boldsymbol{n}}$ and $\vec{\boldsymbol{w}}$, the DMN is trained on linear elastic data alone by solving the optimization problem

$$J\left(\vec{\boldsymbol{n}}, \vec{\boldsymbol{w}}\right) := \frac{1}{N} \sqrt[q]{\sum_{s=1}^{N} \left(\frac{\left\| \bar{\mathbb{C}}^s - \mathcal{DMN}^{\mathcal{L}}\left(\mathbb{C}_1, \mathbb{C}_2, \vec{\boldsymbol{n}}, \vec{\boldsymbol{w}}\right) \right\|_p}{\left\| \bar{\mathbb{C}}^s \right\|_p} \right)^q} + \lambda \left(\sum_{i=1}^{2^K} w_{K+1}^i - 1 \right)^2 \longrightarrow \min_{\vec{\boldsymbol{n}}, \vec{\boldsymbol{w}}} \quad \text{s.t.} \quad \vec{\boldsymbol{w}} \geq 0. \tag{1}$$

Here, $\mathbb{C}_1$, $\mathbb{C}_2$ denote the sampled linear elastic training data, $\bar{\mathbb{C}}$ the computed effective stiffness, and $\mathcal{DMN}^{\mathcal{L}}\left(\mathbb{C}_1, \mathbb{C}_2, \vec{\boldsymbol{n}}, \vec{\boldsymbol{w}}\right)$ represents the DMN's linear elastic homogenization function. Fig. 1(a) illustrates the propagation of input stiffnesses $\mathbb{C}_1$, $\mathbb{C}_2$ through the binary tree to obtain the predicted effective stiffness. After the training, i.e., during the online evaluation, the free parameters $\vec{\boldsymbol{n}}$, $\vec{\boldsymbol{w}}$ remain fixed, and the DMN's predicted effective stress $\bar{\boldsymbol{\sigma}}$ is computed for nonlinear constituent materials by solving the balance of linear momentum in every laminate simultaneously.

3 Numerical results

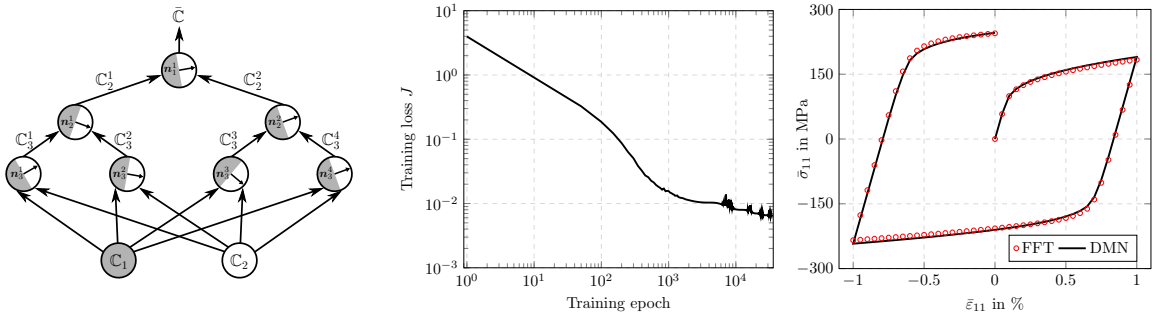
As an example, we investigate a connecting rod made from a metal matrix composite [5], see Fig. 2. The microstructure of the metal matrix composite comprises 30 vol-% linear elastic ceramic particles ($E = 400\,\text{GPa}$, $\nu = 0.2$), embedded into an aluminium matrix, which we assume to be governed by J_2-elastoplasticiy with power-law hardening

$$\sigma_\text{Y} = \sigma_0 + k\varepsilon_\text{p}^m \tag{2}$$

and with $E = 75\,\text{GPa}$, $\nu = 0.3$, $\sigma_\text{Y} = 75\,\text{MPa}$, $k = 416\,\text{MPa}$ and $m = 0.3895$.

* Corresponding author: e-mail sebastian.gajek@kit.edu, phone +49 721 608 46904

First, we sample $N = 800$ tuples of (orthotropic) input stiffnesses $\{(\mathbb{C}_1^s, \mathbb{C}_2^s)\}_{s=1}^N$ and compute the corresponding effective stiffnesses $\bar{\mathbb{C}}^s$ with an FFT-based computational homogenization code [6]. We train a deep material network with $K = 8$ layers for 36 000 epochs by means of accelerated stochastic gradient descent [7]. In Fig. 1(b), the loss J over the training epochs is shown. We observe that the loss is decreasing in a non-monotonic fashion due to a learning rate modulation commonly used in machine learning.



(a) Two-phase direct DMN of depth three **(b)** Loss vs. epochs **(c)** Effective stress vs. effective strain

Fig. 1: A two-phase direct DMN and results for the offline training and the online evaluation

After the training, we assign the above mentioned material behavior to the ceramic inclusions and the aluminum matrix and investigate the effective response of the considered metal matrix composite on the microscopic level. We compute the effective stress with an FFT-based computational homogenization code [6] and compare the former to the effective stress predicted by the DMN. In the 11-direction, a complete stress-strain hysteresis is simulated with a strain amplitude of $\bar{\varepsilon} = 1\%$ in 80 equidistant load steps, see Fig. 1(c). As can be observed, the DMN is able to predict the strongly nonlinear effective stress of the metal matrix composite with reasonable error. Regarding the computational costs, the DMN is able to provide a speed-up over the FFT-based computational homogenization code by a factor of 10^5.

In the next step, we turn our attention to a component-scale simulation of industrial complexity. We implement the DMN as an implicit user-material (UMAT) subroutine in ABAQUS. We mesh the connecting rod by 120 000 quadratic tetrahedron elements. At each Gauss point, a DMN is integrated implicitly. We apply a load of $F = 20$ kN in 10 equidistant loading steps. We observe a stable convergence behavior of the FE simulation, requiring 19 total Newton iterations. The former does not come as a surprise, since the algorithmic tangent of the DMN is computed analytically. Computing on 96 threads in parallel, the simulation takes about 20 minutes to complete, requiring about 18 GB of DRAM.

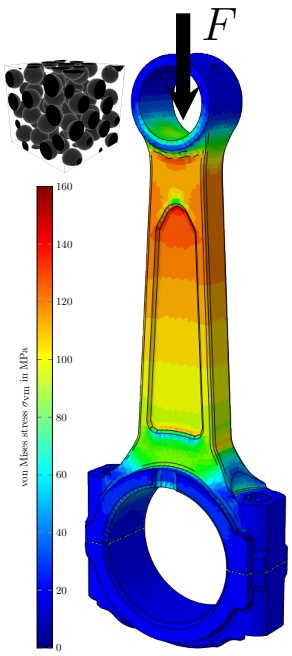


Fig. 2: Von Mises stress distribution in a concurrent two-scale simulation of a connecting rod made from a metal matrix composite. At every Gauss point, a DMN is solved implicitly.

4 Conclusion

Our results indicate that deep material networks enable two-scale simulations of structures with industrial complexity with moderate hardware requirements. In this way, the FE-DMN method represents a strong candidate for realizing concurrent multiscale simulations for industrial applications.

Acknowledgements SG, MS and TB acknowledge financial support by the German Research Foundation (DFG) within the International Research Training Group "Integrated engineering of continuous-discontinuous long fiber reinforced polymer structures" (GRK 2078/2). The support by the DFG is gratefully acknowledged. Open access funding enabled and organized by Projekt DEAL.

References

[1] Z. Liu, C. T. Wu and M. Koishi, Comput. Methods Appl. Mech. Engrg., **345**, 1138–1168, (2019)
[2] Z. Liu and C. T. Wu, J. Mech. Phys. Solids, **127**, 20–46, (2019)
[3] S. Gajek, M. Schneider and Thomas Böhlke, J. Mech. Phys. Solids, **142**, 103984, (2020)
[4] S. Gajek, M. Schneider and Thomas Böhlke, arXiv, **2103.08253**, (2021)
[5] J. Segurado and J. Llorca and C. González, Scr. Mater., **46**, 525–529, (2002)
[6] H. Moulinec and P. Suquet, C. R. Acad. Sci., **318**, 1417–1423, (1994)
[7] D. P. Kingma and J. Ba, 3rd ICLR, (2015)

