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**Transfer learning of deep material network for seamless structure-property predictions.**  
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Summary: Modern materials design requires reliable and consistent structure-property relationships. The paper addresses the need through transfer learning of deep material network (DMN). In the proposed learning strategy, we store the knowledge of a pre-trained network and reuse it to generate the initial structure for a new material via a naive approach. Significant improvements in the training accuracy and learning convergence are attained. Since all the databases share the same base network structure, their fitting parameters can be interpolated to seamlessly create intermediate databases. The new transferred models are shown to outperform the analytical micromechanics methods in predicting the volume fraction effects. We then apply the unified DMN databases to the design of failure properties, where the failure criteria are defined upon the distribution of microscale plastic strains. The Pareto frontier of toughness and ultimate tensile strength is extracted from a large-scale design space enabled by the efficiency of DMN extrapolation.

**MSC:**

74 Mechanics of deformable solids

**Keywords:**

[multiscale modeling](#); [machine learning](#); [micromechanics](#); [nonlinear plasticity](#); [failure analysis](#); [materials design](#)

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**References:**

- [1] Olson, GB, Computational design of hierarchically structured materials, *Science*, 277, 1237-1242, (1997)
- [2] Panchal, JH; Kalidindi, SR; McDowell, DL, Key computational modeling issues in integrated computational materials engineering, *Comput Aided Des*, 45, 4-25, (2013)
- [3] McVeigh, C.; Vernerey, F.; Liu, WK; Brinson, LC, Multiresolution analysis for material design, *Comput Methods Appl Mech Eng*, 195, 5053-5076, (2006) · [Zbl 1118.74040](#)
- [4] Buljac, A.; Jailin, C.; Mendoza, A.; Neggers, J.; Taillandier-Thomas, T.; Bouterf, A.; Smaniotto, B.; Hild, F.; Roux, S., Digital volume correlation: review of progress and challenges, *Exp Mech*, 58, 661-708, (2018)
- [5] Hill, R., Elastic properties of reinforced solids: some theoretical principles, *J Mech Phys Solids*, 11, 357-372, (1963) · [Zbl 0114.15804](#)
- [6] Feyel, F.; Chaboche, JL, FE2 multiscale approach for modelling the elastoviscoplastic behaviour of long fibre SIC/TI composite materials, *Comput Methods Appl Mech Eng*, 183, 309-330, (2000) · [Zbl 0993.74062](#)
- [7] Wu, CT; Koishi, M., Three-dimensional meshfree-enriched finite element formulation for micromechanical hyperelastic modeling of particulate rubber composites, *Int J Numer Methods Eng*, 91, 1137-1157, (2012)
- [8] Wu, CT; Guo, Y.; Askari, E., Numerical modeling of composite solids using an immersed meshfree Galerkin method, *Compos Part B Eng*, 45, 1397-1413, (2013)
- [9] Moulinec, H.; Suquet, P., A numerical method for computing the overall response of nonlinear composites with complex microstructure, *Comput Methods Appl Mech Eng*, 157, 69-94, (1998) · [Zbl 0954.74079](#)
- [10] Geus, T.; Vondřejc, J.; Zeman, J.; Peerlings, R.; Geers, M., Finite strain FFT-based non-linear solvers made simple, *Comput Methods Appl Mech Eng*, 318, 412-430, (2017)
- [11] Yvonnet, J.; Monteiro, E.; He, QC, Computational homogenization method and reduced database model for hyperelastic heterogeneous structures, *Int J Multiscale Comput Eng*, 11, 201-225, (2013)
- [12] Yang, Z.; Yabansu, YC; Al-Bahrani, R.; Liao, Wk; Choudhary, AN; Kalidindi, SR; Agrawal, A., Deep learning approaches for mining structure – property linkages in high contrast composites from simulation datasets, *Comput Mater Sci*, 151, 278-287, (2018)
- [13] Bessa, M.; Bostanabad, R.; Liu, Z.; Hu, A.; Apley, D.; Brinson, C.; Chen, W.; Liu, W., A framework for data-driven analysis of materials under uncertainty: countering the curse of dimensionality, *Computer Methods Appl Mech Eng*, 320, 633-667,

(2017)

- [14] Raissi, M.; Karniadakis, GE, Hidden physics models: machine learning of nonlinear partial differential equations, *J Comput Phys*, 357, 125-141, (2018) · [Zbl 1381.68248](#)
- [15] Chen, Z.; Huang, T.; Shao, Y.; Li, Y.; Xu, H.; Avery, K.; Zeng, D.; Chen, W.; Su, X., Multiscale finite element modeling of sheet molding compound (smc) composite structure based on stochastic mesostructure reconstruction, *Compos Struct*, 188, 25-38, (2018)
- [16] Oliver, J.; Caicedo, M.; Huespe, A.; Hernández, J.; Roubin, E., Reduced order modeling strategies for computational multiscale fracture, *Computer Methods Appl Mech Eng*, 313, 560-595, (2017)
- [17] Kalidindi SR (2015) *Hierarchical materials informatics: novel analytics for materials data*. Elsevier, Amsterdam
- [18] Latypov, MI; Toth, LS; Kalidindi, SR, Materials knowledge system for nonlinear composites, *Computer Methods Appl Mech Eng*, 346, 180-196, (2019)
- [19] Liu, Z.; Bessa, M.; Liu, WK, Self-consistent clustering analysis: an efficient multi-scale scheme for inelastic heterogeneous materials, *Computer Methods Appl Mech Eng*, 306, 319-341, (2016)
- [20] Liu, Z.; Fleming, M.; Liu, WK, Microstructural material database for self-consistent clustering analysis of elastoplastic strain softening materials, *Computer Methods Appl Mech Eng*, 330, 547-577, (2018)
- [21] Liu Z, Kafka OL, Yu C, Liu WK (2018) Data-driven self-consistent clustering analysis of heterogeneous materials with crystal plasticity. In: *Advances in computational plasticity*. Springer, pp 221-242
- [22] Yu, C.; Kafka, OL; Liu, WK, Self-consistent clustering analysis for multiscale modeling at finite strains, *Computer Methods Appl Mech Eng*, 349, 339-359, (2019)
- [23] Liu, Z.; Wu, C.; Koishi, M., A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials, *Computer Methods Appl Mech Eng*, 345, 1138-1168, (2019)
- [24] Liu, Z.; Wu, C., Exploring the 3d architectures of deep material network in data-driven multiscale mechanics, *J Mech Phys Solids*, 127, 20-46, (2019)
- [25] Thrun S (1996) Is learning the n-th thing any easier than learning the first? In: *Advances in neural information processing systems*, pp 640-646
- [26] Raina R, Ng AY, Koller D (2006) Constructing informative priors using transfer learning. In: *Proceedings of the 23rd international conference on machine learning*. ACM, pp 713-720
- [27] Lubbers, N.; Lookman, T.; Barros, K., Inferring low-dimensional microstructure representations using convolutional neural networks, *Phys Rev E*, 96, 052111, (2017)
- [28] Simonyan K, Zisserman A (2014) Very deep convolutional networks for large-scale image recognition. *arXiv preprint arXiv:1409.1556*
- [29] Li, X.; Zhang, Y.; Zhao, H.; Burkhart, C.; Brinson, LC; Chen, W., A transfer learning approach for microstructure reconstruction and structure – property predictions, *Sci Rep*, 8, 13461, (2018)
- [30] Melro, A.; Camanho, P.; Pinho, S., Generation of random distribution of fibres in long-fibre reinforced composites, *Compos Sci Technol*, 68, 2092-2102, (2008)
- [31] Mori, T.; Tanaka, K., Average stress in matrix and average elastic energy of materials with misfitting inclusions, *Acta Metall*, 21, 571-574, (1973)
- [32] Hill, R., A self-consistent mechanics of composite materials, *J Mech Phys Solids*, 13, 213-222, (1965)
- [33] Eshelby, JD, The determination of the elastic field of an ellipsoidal inclusion, and related problems, *Proc R Soc Lond A*, 241, 376-396, (1957) · [Zbl 0079.39606](#)
- [34] Christensen, R.; Lo, K., Solutions for effective shear properties in three phase sphere and cylinder models, *J Mech Phys Solids*, 27, 315-330, (1979) · [Zbl 0419.73007](#)

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