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**A deep material network for multiscale topology learning and accelerated nonlinear modeling of heterogeneous materials.** (English) Zbl 1440.74340  
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Summary: In this paper, a new data-driven multiscale material modeling method, which we refer to as deep material network, is developed based on mechanistic homogenization theory of representative volume element (RVE) and advanced machine learning techniques. We propose to use a collection of connected mechanistic building blocks with analytical homogenization solutions to describe complex overall material responses which avoids the loss of essential physics in generic neural network. This concept is demonstrated for 2-dimensional RVE problems and network depth up to 7. Based on linear elastic RVE data from offline direct numerical simulations, the material network can be effectively trained using stochastic gradient descent with backpropagation algorithm, further enhanced by model compression methods. Importantly, the trained network is valid for any local material laws without the need for additional calibration or micromechanics assumption. Its extrapolations to unknown material and loading spaces for a wide range of problems are validated through numerical experiments, including linear elasticity with high contrast of phase properties, nonlinear history-dependent plasticity and finite-strain hyperelasticity under large deformations. By discovering a proper topological representation of RVE with fewer degrees of freedom, this intelligent material model is believed to open new possibilities of high-fidelity efficient concurrent simulations for a large-scale heterogeneous structure. It also provides a mechanistic understanding of structure – property relations across material length scales and enables the development of parameterized microstructural database for material design and manufacturing.

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**MSC:**

**74Q05** Homogenization in equilibrium problems of solid mechanics

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[material network](#); [building blocks](#); [machine learning](#); [nonlinear plasticity](#); [large deformations](#)

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**References:**

- [1] Hill, R., A self-consistent mechanics of composite materials, *J. Mech. Phys. Solids*, 13, 4, 213-222 (1965)
- [2] Feyel, F.; Chaboche, J.-L., Fe 2 multiscale approach for modelling the elastoviscoplastic behaviour of long fibre sic/ti composite materials, *Comput. Methods Appl. Mech. Engrg.*, 183, 3, 309-330 (2000)
- [3] Geers, M. G.; Kouznetsova, V. G.; Brekelmans, W., Multi-scale computational homogenization: Trends and challenges, *J. Comput. Appl. Math.*, 234, 7, 2175-2182 (2010)
- [4] Belytschko, T.; Loehnert, S.; Song, J.-H., Multiscale aggregating discontinuities: A method for circumventing loss of material stability, *Internat. J. Numer. Methods Engrg.*, 73, 6, 869-894 (2008)
- [5] Wu, C. T.; Koishi, M., Three-dimensional meshfree-enriched finite element formulation for micromechanical hyperelastic modeling of particulate rubber composites, *Internat. J. Numer. Methods Engrg.*, 91, 11, 1137-1157 (2012)
- [6] Wu, C. T.; Wang, D.; Guo, Y., An immersed particle modeling technique for the three-dimensional large strain simulation of particulate-reinforced metal-matrix composites, *Appl. Math. Model.*, 40, 4, 2500-2513 (2016)
- [7] Moulinec, H.; Suquet, P., A numerical method for computing the overall response of nonlinear composites with complex microstructure, *Comput. Methods Appl. Mech. Engrg.*, 157, 1-2, 69-94 (1998)
- [8] De Geus, T.; Vondřejc, J.; Zeman, J.; Peerlings, R.; Geers, M., Finite strain fft-based non-linear solvers made simple, *Comput. Methods Appl. Mech. Engrg.*, 318, 412-430 (2017)
- [9] Eshelby, J. D., The determination of the elastic field of an ellipsoidal inclusion, and related problems, *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, 241, 1226, 376-396 (1957)
- [10] Hashin, Z.; Shtrikman, S., A variational approach to the theory of the elastic behaviour of multiphase materials, *J. Mech. Phys. Solids*, 11, 2, 127-140 (1963)

- [11] Mura, T., *Micromechanics of Defects in Solids*, Vol. 3 (1987), Springer Science & Business Media
- [12] Liu, Z.; Moore, J. A.; Aldousari, S. M.; Hedia, H. S.; Asiri, S. A.; Liu, W. K., A statistical descriptor based volume-integral micromechanics model of heterogeneous material with arbitrary inclusion shape, *Comput. Mech.*, 1-19 (2015)
- [13] Liu, Z.; Moore, J. A.; Liu, W. K., An extended micromechanics method for probing interphase properties in polymer nanocomposites, *J. Mech. Phys. Solids*, 95, 663-680 (2016)
- [14] Bhattacharjee, S.; Matouš, K., A nonlinear manifold-based reduced order model for multiscale analysis of heterogeneous hyperelastic materials, *J. Comput. Phys.*, 313, 635-653 (2016)
- [15] Michel, J.; Suquet, P., Nonuniform transformation field analysis, *Int. J. Solids Struct.*, 40, 25, 6937-6955 (2003), special issue in Honor of George J. Dvorak
- [16] Michel, J.-C.; Suquet, P., A model-reduction approach in micromechanics of materials preserving the variational structure of constitutive relations, *J. Mech. Phys. Solids*, 90, 254-285 (2016)
- [17] Jolliffe, I., *Principal Component Analysis* (2002), Wiley Online Library
- [18] Yvonnet, J.; He, Q.-C., The reduced model multiscale method (r3m) for the non-linear homogenization of hyperelastic media at finite strains, *J. Comput. Phys.*, 223, 1, 341-368 (2007)
- [19] Kerfriden, P.; Goury, O.; Rabczuk, T.; Bordas, S. P.-A., A partitioned model order reduction approach to rationalise computational expenses in nonlinear fracture mechanics, *Comput. Methods Appl. Mech. Engrg.*, 256, 169-188 (2013)
- [20] Oliver, J.; Caicedo, M.; Huespe, A.; Hernández, J.; Roubin, E., Reduced order modeling strategies for computational multiscale fracture, *Comput. Methods Appl. Mech. Engrg.*, 313, 560-595 (2017)
- [21] Liu, Z.; Bessa, M.; Liu, W. K., Self-consistent clustering analysis: An efficient multi-scale scheme for inelastic heterogeneous materials, *Comput. Methods Appl. Mech. Engrg.*, 306, 319-341 (2016)
- [22] Liu, Z.; Fleming, M.; Liu, W. K., Microstructural material database for self-consistent clustering analysis of elastoplastic strain softening materials, *Comput. Methods Appl. Mech. Engrg.*, 330, 547-577 (2018)
- [23] Hinton, G.; Deng, L.; Yu, D.; Dahl, G. E.; Mohamed, A.-r.; Jaitly, N.; Senior, A.; Vanhoucke, V.; Nguyen, P.; Sainath, T. N., Deep neural networks for acoustic modeling in speech recognition: The shared views of four research groups, *IEEE Signal Process. Mag.*, 29, 6, 82-97 (2012)
- [24] LeCun, Y.; Bengio, Y.; Hinton, G., Deep learning, *Nature*, 521, 7553, 436 (2015)
- [25] Goodfellow, I.; Bengio, Y.; Courville, A., *Deep Learning* (2016), MIT Press
- [26] Silver, D.; Schrittwieser, J.; Simonyan, K.; Antonoglou, I.; Huang, A.; Guez, A.; Hubert, T.; Baker, L.; Lai, M.; Bolton, A., Mastering the game of go without human knowledge, *Nature*, 550, 7676, 354 (2017)
- [27] Le, B.; Yvonnet, J.; He, Q.-C., Computational homogenization of nonlinear elastic materials using neural networks, *Internat. J. Numer. Methods Engrg.*, 104, 12, 1061-1084 (2015)
- [28] Yvonnet, J.; Monteiro, E.; He, Q.-C., Computational homogenization method and reduced database model for hyperelastic heterogeneous structures, *Int. J. Multiscale Comput. Eng.*, 11, 3, 201-225 (2013)
- [29] Bessa, M.; Bostanabad, R.; Liu, L.; 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, *Comput. Methods Appl. Mech. Engrg.*, 320, 633-667 (2017)
- [30] Ibañez, R.; Borzacchiello, D.; Aguado, J. V.; Abisset-Chavanne, E.; Cueto, E.; Ladevèze, P.; Chinesta, F., Data-driven non-linear elasticity: constitutive manifold construction and problem discretization, *Comput. Mech.*, 60, 5, 813-826 (2017)
- [31] Ghaboussi, J.; Garrett Jr, J.; Wu, X., Knowledge-based modeling of material behavior with neural networks, *J. Eng. Mech.*, 117, 1, 132-153 (1991)
- [32] Unger, J. F.; Könke, C., Coupling of scales in a multiscale simulation using neural networks, *Comput. Struct.*, 86, 21-22, 1994-2003 (2008)
- [33] Wang, K.; Sun, W., A multiscale multi-permeability poroplasticity model linked by recursive homogenizations and deep learning, *Comput. Methods Appl. Mech. Engrg.*, 334, 337-380 (2018)
- [34] Glorot, X.; Bordes, A.; Bengio, Y., Deep sparse rectifier neural networks, (*Proceedings of the Fourteenth International Conference on Artificial Intelligence and Statistics* (2011)), 315-323
- [35] Cahn, J. W.; Hilliard, J. E., Free energy of a nonuniform system. i. interfacial free energy, *J. Chem. Phys.*, 28, 2, 258-267 (1958)
- [36] Choromanska, A.; Henaff, M.; Mathieu, M.; Arous, G. B.; LeCun, Y., The loss surfaces of multilayer networks, (*Artificial Intelligence and Statistics* (2015)), 192-204
- [37] Dvorak, G. J., Transformation field analysis of inelastic composite materials, *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, 437, 1900, 311-327 (1992)

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