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Physics-guided neural networks for constitutive modeling and nonlinear multiscale simulation

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Efficient multiscale simulation of finite deformations of soft composites and metamaterials requires the homogenization of effective constitutive models from microstructural simulations. Such effective material models must comply with continuum mechanical requirements, i.e., the laws of thermodynamics, material frame indifference, material symmetry, growth conditions, and ellipticity. While analytical models may not be able to capture the highly nonlinear behavior of soft microstructures such as beam lattices, data-driven models are more flexible, but so far they do not consider all requirements. In this work, we present a data-driven constitutive modeling framework for the multiscale simulation of microstructured materials, which conforms to the physical model requirements by construction. The strain energy function is formulated as an input-convex feed-forward neural network to fulfill the polyconvexity condition, which implies ellipticity. Two approaches are introduced: A model based on a set of polyconvex, anisotropic and objective invariants, and a highly flexible model that is formulated in terms of the deformation gradient, its cofactor and determinant. When calibrated with the challenging homogenization data of cubic beam lattices with instabilities, the invariant-based model shows drawbacks for several deformation modes. The model based on the deformation gradient alone is able to reproduce and predict the effective material behavior very well. Only a moderate amount of physically motivated calibration data is used, which shows the excellent generalization capabilities of these physics-guided data-driven constitutive models. Subsequently, the application in sequential multiscale simulations and the extension towards parametric, inelastic and multi-physical materials are discussed.