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Two-stage data-driven homogenization for nonlinear solids using a reduced order model

Abstract. The nonlinear behavior of materials with three-dimensional microstructure is investigated using a data-driven approach. The key innovation is the combination of two hierarchies of precomputations with sensibly chosen sampling sites and adapted interpolation functions: First, finite element (FE) simulations are performed on the microstructural level. A sophisticated sampling strategy is developed in order to keep the number of costly FE computations low. Second, the generated simulation data serves as input for a reduced order model (ROM). The ROM allows for considerable speed-ups on the order of 10-100. Still, its performance is below the demands for actual twoscale simulations. In order to attain the needed speed-ups, in a third step, the use of radial numerically explicit potentials (RNEXP) is proposed. The latter combine uni-directional cubic interpolation functions with radial basis functions operating on geodesic distances. The evaluation of the RNEXP approximation is realized almost in real-time. It benefits from the computational efficiency of the ROM since a higher number of sampling points can be realized than if direct FE simulations were used. By virtue of the dedicated sampling strategy less samples and, thus, precomputations (both FE and ROM) are needed than in competing techniques from literature. These measures render the offline cost of the RNEXP manageable on workstation computers. Additionally, the chosen sampling directions show favorable for the employed kernel interpolation. Numerical examples for highly nonlinear hyperelastic (pseudo-plastic) composite materials with isotropic and anisotropic microstructure are investigated. Twoscale simulations involving more than 10^6 DOF on the structural level are solved using the RNEXP and the influence of the microstructure on the structural behavior is quantified.

Keywords: reduced order model; data-driven computational homogenization; RNEXP

1 Introduction

The aim of homogenization methods is the prediction of the effective properties of microstructured solids. Examples for such materials are particle or fiber reinforced thermoplastics, porous metals, foams and polycrystalline solids. Many promising methods have been suggested which extend the early first order estimates proposed by Voigt [1] and Reuss [2]. For linear materials estimates and bounds of various type have been proposed, e.g. the well-known upper and lower Hashin-Shtrikman bounds [3]. Various monographs on the topic have been published (e.g. [4; 5]). For nonlinear materials the estimation is more difficult, especially when path-dependent problems are considered (see, e.g., [6; 7] for review articles). The simple first order Taylor and Sachs estimates lead to overly stiff or soft predictions. Variational estimates can achieve better accuracy (e.g. [8; 9; 10]), but are more involved. For specific applications the general homogenization problem is often specialized, e.g. in the Gurson model [11] for porous metals and the many extensions thereof (e.g. [12; 13]).

While analytical methods are often useful in the presence of isotropic microstructures or simple topologies and morphologies (e.g. spheroids with specific orientation distribution), computational methods can help to predict the material behavior in the presence of more complicated microstructures. Simulations can provide reliable information on the hardening and damaging behavior and they can predict viscous effects. For solid mechanical problems the finite element method (FEM) can be considered as the method of choice for general problems although schemes based on the Fast Fourier Transform (FFT) are seeing increasing attention for homogenization problems, e.g. [14].

A short-coming of the FEM (and more general of simulation methods) is their high computational cost: each simulation requires billions of algebraic operations and produces a lot of information that often needs to be stored (e.g. history variables). For instance the numerical studies presented for porous materials in [15] dealt with rather simple materials but required massive computational resources. In order to alleviate the computational burden, reduced order models have become rather fashionable, especially in the context of nonlinear homogenization. A major development in this direction was the Nonuniform Transformation Field Analysis (NTFA, [16; 17]). Later the NTFA has been extended in terms of the potential-based reduced basis model order reduction (pRBMOR) of the authors [18]. The