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# Reduced order modeling in nonlinear homogenization: A comparative study



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#### ABSTRACT

Computationally inexpensive nonlinear homogenization methods are much sought after in academia and industry. However, the accuracy and the accessibility of the methods play an important role. Two nonlinear homogenization methods for microstructured solid materials are investigated in this work: the pRBMOR (Fritzen and Leuschner, 2013; Fritzen et al., 2014) and the NUTFA (Sepe et al., 2013). Both methods are based on ideas of the nonuniform transformation field analysis (NTFA; Michel and Suquet, 2003, 2004). A detailed comparison with respect to accuracy, storage requirements and the evolution of the reduced degrees of freedom is carried out. Numerical examples for two- and three-dimensional problems undergoing nonproportional load paths are presented.

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#### 1. Introduction

Heterogeneous composite materials are obtained by combining two or more different materials in order to produce new materials that are unique in terms of their physical properties. The main objective in composite design is to combine the favorable properties of the individual constituents in order to complement each other, e.g., in order to complement high strength with ductility or with low specific weight. The resulting material then has advantageous overall characteristics, which enable superior structural performance over designs relying on the individual phases. Therefore, composite materials have become the dominant materials in various fields of engineering over the last years. Additionally, composites can also allow for novel manufacturing processes that can help to reduce production cost significantly, e.g. in the sense of short fiber reinforced thermoplastics. Thereby, composites have helped to revolutionize traditional design concepts. They led to a wide range of innovative applications.

In order to allow for reliable mechanical designs the material properties of composite materials need to be characterized with full account of the micro-heterogeneities. The consideration of the heterogeneities is required as they significantly influence the structural response. Important microstructural characteristics include, e.g., the phase volume fractions and the shape and orientation of inclusion phases. Several methods have been proposed in the literature with the aim of predicting the properties of linear (thermo-)elastic microheterogeneous materials [e.g., 6–9]. A branch of homogenization has focused on the estimation of rigorous bounds for the effective properties of linear and, later, nonlinear composites using variational methods [e.g., 10–14]. Computational methods for the prediction of the linear properties of materials can be considered standard procedures today [see, e.g., 15,16].

In practice, many engineering composites are made of constituents showing an effective nonlinear behavior induced by inelastic phenomena occurring at the microscale. Thus, it is required to understand the mechanisms acting on the microscale in order to predict the overall behavior of the material. This makes the prediction of the mechanical response of a heterogeneous medium whose constituents are characterized by inelastic phenomena such as plasticity, damage, and viscous effects, a highly non-trivial task.

The computational homogenization method [also FE<sup>2</sup>; e.g., 17–19] has been increasingly used in the academic community during the last years. It allows for an accurate approximation of the actual nonlinear effective behavior of heterogeneous materials.

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However, these numerical techniques involve a large number of internal variables, many degrees of freedom and, thus, lead to a prohibitively high computational burden in terms of memory usage and computing time. One way to realize three-dimensional twoscale simulations involving nonlinear composites is to use model order reduction techniques. These should be reasonably accurate and computationally efficient at the same time. The idea of these methods is to reduce the great amount of information that exists at the microscopic scale in a systematic way, with the aim of finding approximations leading to computationally viable methods. This has led to simplified homogenization approaches reducing the computational complexity of the micromechanical simulations.

One important nonlinear micromechanical homogenization method is the Transformation Field Analysis (TFA) initially proposed by Dvorak [20]. The TFA represents an elegant way for reducing the number of the macroscopic internal variables by considering the microscopic field of internal variables to be piecewise uniform. In particular, it considers the inelastic strain as a given eigenstrain that leads to characteristic eigendeformations and associated stress states which are computed numerically. The evolution of the internal variables within each constituent then stems from the mean stress on the sub-domain. This makes the method a hybrid homogenization method combining numerical methods (for the determination of the eigensolutions) and analytical approaches (resulting in the evolution laws for the piecewise uniform internal variables).

The TFA method was extended, e.g., by Fish et al. [21] to periodic composites and it has been utilized successfully for structural computations by various authors [22-27]. Furthermore, the TFA method was improved by Dvorak et al. [22] who proposed a piece-wise uniform TFA (PWUTFA) subdividing each material phase into several subsets. Chaboche et al. [28] developed a PWUTFA in order to derive the nonlinear behavior of damaging composite materials. Later, Chaboche et al. [29] proposed a corrected TFA that can help to reduce the number of sub-domains while preserving a sufficient accuracy. Still, the assumption of piecewise uniform inelastic strains is overly restrictive and, e.g., cannot lead to precise predictions of the local fields without an important increase of the computational complexity (via an increasing number of sub-domains). This has been observed by Suguet [30]; Michel et al. [31], where the PWUTFA applied to two-phase composites may require the subdivision of each material phase into numerous sub-domains in order to obtain an accurate description of the effective response of the composite. This is due to the intrinsic nonuniformity of the inelastic strain field even within a single material constituent. Generally, too few sub-domains lead to an overestimation of the stresses. Since the number of the sub-domains and the number of reduced variables depend linearly on each other, the number of reduced variables can easily get prohibitively high if a reasonable accuracy in the effective constitutive relations is required.

In order to properly reproduce the mechanical response of the representative volume element of a nonlinear composite it is, important to capture the heterogeneity of the inelastic strain field. This observation has motivated the development of the Nonuniform Transformation Field Analysis (NTFA) introduced by Michel and Suquet [4]. The inelastic strain within each material phase is considered as nonuniform and described as the superposition of tensorial functions called inelastic modes. The modes are extracted from snapshots of nonlinear simulations of the composite along pre-defined loading paths during a pre-analysis stage. It shall be noted that the hardening variables are still assumed to be piecewise uniform, and that the evolution of the reduced internal variables can only partially be motivated from micromechanics.

The NTFA method was implemented for the study of nonlinear composite materials with rate-dependent (elasto-viscoplastic) constituents or rate-independent (elasto-plastic) constituents by Michel and Suquet [5]. Franciosi and Berbenni [32,33] used an affiliated approach for the modeling of heterogeneous crystal and poly-crystal plasticity, characterized by hierarchical multi-laminate structures. Another application for elasto-viscoplastic and porous elasto-viscoplastic constituents was given by Roussette et al. [34], where the snapshot POD was used for the first time in order to systematically extract the most significant plastic strain modes. All these applications focused on two-dimensional investigations using the Fast Fourier Transform [FFT, e.g., 35-37]. In order to tackle more realistic three-dimensional problems, Fritzen and Böhlke [38] proposed a first application of the NTFA for three-dimensional problems using the finite element method. Later, the NTFA was used by Fritzen and Böhlke [39] for the analysis of the impact of the morphological anisotropy of inclusions in nonlinear metal ceramic composites. A micromechanically motivated extension of the NTFA for linear viscoelastic materials was given by Fritzen and Böhlke [40]. The latter work involved also several analytical results based on the computationally defined viscoelastic modes that emphasize the hybrid (computational and micromechanical) character of the approach. Another application to sophisticated viscoelastic problems including swelling and aging was recently published by Largenton et al. [41].

Marfia and Sacco [42] presented a PWUTFA homogenization procedure for the multiscale analysis of periodic masonry, assuming a bilinear approximation for the inelastic strain of one subset of the unit cell. Sepe et al. [3] proposed a non uniform transformation field analysis (NUTFA) for studying composites with plastic and shape memory alloy constituents. It differs from the NTFA proposed by Michel and Suquet [4] for what concerns the approximation of the inelastic strains and the evolution of the reduced variables.

The aim of the current work is to present and compare two different reduced basis methods for the solution of the nonlinear homogenization problem: the mixed incremental variational approach of Fritzen and Leuschner [pRBMOR: 1]. Fritzen et al. [2] and the projection based approach introduced by Sepe et al. [3]. Both methods are conceived in the NTFA framework but differ with respect to the definition of the inelastic modes and via the definition of the evolution of the internal variables. In the pRBMOR proposed by Fritzen and Leuschner [1]; Fritzen et al. [2], the inelastic modes are determined based on inelastic pre-computations using a full discretization of the microscopic domain and a set of pre-defined loadings; in the approach presented in Sepe et al. [3] they are pre-defined analytical functions that are not subject to a priori defined constraints. Further, the evolution of the reduced degrees of freedom is significantly different for the two approaches. In the current contribution a detailed comparison of advantages and disadvantages of the two methodologies is presented. Numerical applications are carried out for the 2D and 3D analyses of periodic composites subjected to complex loading histories, in order to assess the efficiency of the two methods.

The outline of the paper is as follows: in Section 2 the homogenization problem is introduced. The two reduced order homogenization methods are described in Section 3. The numerical results for the different benchmark problems are presented and compared in Section 4. Section 5 provides a concise summary and concluding remarks.

#### 1.1. General notation

An index-free notation is adopted with scalar quantities typeset as lowercase Latin and Greek letters (e.g.:  $a, n, \psi, \ldots$ ), vectors as bold face lowercase letters (e.g.,  $a, n, \ldots$ ) and second-order tensors as bold face Greek or uppercase Latin letters (e.g.,  $\varepsilon, \sigma, A$ ).

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