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Self-consistent clustering analysis: An efficient multi-scale scheme for inelastic heterogeneous materials

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Abstract

The discovery of efficient and accurate descriptions for the macroscopic behavior of materials with complex microstructure is an outstanding challenge in mechanics of materials. A mechanistic, data-driven, two-scale approach is developed for predicting the behavior of general heterogeneous materials under irreversible processes such as inelastic deformation. The proposed approach includes two major innovations: (1) the use of a data compression algorithm, k-means clustering, during the offline stage of the method to homogenize the local features of the material microstructure into a group of clusters; and (2) a new method called self-consistent clustering analysis used in the online stage that is valid for any local plasticity laws of each material phase without the need for additional calibration. A particularly important feature of the proposed approach is that the offline stage only uses the linear elastic properties of each material phase, making it efficient. This work is believed to open new avenues in parameter-free multi-scale modeling of complex materials, and perhaps in other fields that require homogenization of irreversible processes.

Keywords: Multi-scale; Reduced order model; Plasticity; Data compression; k-means clustering; Self-consistent method

1. Introduction

Materials are hierarchical in nature, involving an inter-play between simple small-scale constituents that together form elaborate compounds that can span multiple time- and length-scales. This multi-scale nature of heterogeneous materials poses a continuing challenge in computational modeling of macroscopic structures. Ideally, efficient and accurate predictions of the macroscopic behavior of heterogeneous materials should be uniquely obtained from the constitutive behavior of each separate constituent (material phase) and from the information about the material microstructure.

Traditional phenomenological constitutive relations [1–3] characterize the average behaviors of the material, i.e. the contributions from all the material phases are not accounted for as an individual interaction of separate constituents.

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These laws regard materials as "black boxes," implying the need for burdensome experimental characterization and tedious calibration. In addition, they are problem-dependent and tend to fail when capturing highly localized microstructure-induced nonlinear material behaviors, such as plasticity, damage and fatigue.

Concurrent multiscale methods [4–11] avoid this calibration process by directly establishing the connection between the microstructure and the macro-response of materials. These concurrent methods link to *every* macroscopic point of a structure a high-fidelity simulation of a Representative Unit Cell (RUC) [12,13] of the microstructure. Since each RUC is already associated to a large computational cost, the total computational cost of this approach is tremendous.

A myriad of methods have been developed with the goal of finding an appropriate balance between cost and accuracy; these are generally referred as reduced order models. Analytical micromechanical methods [14–17], the Voronoi cell finite element method [18], fast Fourier transforms [19], spectral methods [20], the generalized method of cells [21], the transformation field analysis (TFA) [22], the nonuniform transformation field analysis (NTFA) [23,24], the principal component analysis [25–27] or proper orthogonal decomposition[1] (POD) [28–31], and the proper generalized decomposition (PGD) [32–36] are some of the most successful methods of this kind.

Analytical micromechanical methods [14–17] are very efficient because they describe the heterogeneous material by several microstructural descriptors, rather than considering the whole representative unit cell explicitly. However, they are based on mean-field assumptions and linear superposition. This limits their applicability when complex microstructure and localized nonlinear material behavior such as plasticity are present.

POD uses linear combinations of all input variables to define the principal components (modes) to make the predictions for general load cases. This is a fundamental issue when describing nonlinear irreversible plastic processes that is only mitigated by using many snapshots in the offline stage which increases the computational cost of the online stage to unreasonable values [29,37].

The NTFA introduced by Michel and Suquet [23] and further explored by Oskay and Fish [38] among others [39,40], approaches the problem differently with the aim of drastically reducing computational cost [39]. The idea behind NTFA is to leverage the capabilities of analytical micromechanical methods to define a set of reduced variables (e.g. plastic strain fields and internal variables of the local constitutive laws) that are then subjected to "evolution equations" [23,41]. Consequently, the computational cost of NTFA is low but the inclusion of empirical laws that require further calibration is a limitation. Furthermore, the representative unit cells need to be subjected to irreversible deformation to obtain the plastic modes (as in POD) which leads to an extensive exploration of the deformation space at the offline stage.

In this article a new approach is proposed where the above-mentioned limitations are addressed simultaneously by meeting three fundamental goals: (1) avoiding to have an extensive exploratory offline stage (as in NTFA and especially POD), by limiting this stage to the characterization of the *elastic behavior* of the representative unit cell; (2) eliminating the need to find reduced macro-constitutive equations (as in NTFA), i.e. only using the local constitutive equations of each phase present in the representative unit cell without calibration of additional laws; and (3) achieving a reduction in computational time of several orders of magnitude without significantly compromising accuracy.

In order to achieve these goals *two fundamental contributions* are introduced in Section 2: a new analysis method applicable to any reduced RUC; and a procedure based on a data compression algorithm to obtain any reduced RUC. Section 3 shows the results and discusses the accuracy and efficiency of the methodology. Concluding remarks are provided in Section 4.

2. Methodology

The starting point is a high-fidelity Representative Unit Cell (RUC) of the material, i.e. a representative domain of the microstructure of a material. This high-fidelity RUC can be analyzed by different methods, e.g. finite element or meshfree methods, such that accurate predictions of the material's mechanical behavior are achieved. However, the computational cost associated to these RUCs is usually significantly large because they involve a very fine numerical discretization to capture the microstructural shapes of the material and its detailed mechanical behavior.

With the aim of lowering the computational expense one may consider to decompose the high-fidelity RUC into a group of large subdomains, obtaining a reduced RUC— Fig. 1. These subdomains are designated as **material clusters**

[1] The mechanics community refers to principal component analysis as proper orthogonal decomposition (POD).