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Numerical material representation using proper orthogonal decomposition and diffuse approximation

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ABSTRACT

From numerical point of view, analysis and optimization in computational material engineering require efficient approaches for microstructure representation. This paper develops an approach to establish an image-based interpolation model in order to efficiently parameterize microstructures of a representative volume element (RVE), based on proper orthogonal decomposition (POD) reduction of density maps (snapshots). When the parameters of the RVE snapshot are known *a priori*, the geometry and topology of individual phases of a parameterized snapshot is given by a series of response surfaces of the projection coefficients in terms of these parameters. Otherwise, a set of pseudo parameters corresponding to the detected dimensionality of the data set are taken from learning the manifolds of the projection coefficients. We showcase the approach and its potential applications by considering a set of two-phase composite snapshots. The choice of the number of retained modes is made after considering both the image reconstruction errors as well as the convergence of the effective material constitutive behavior obtained by numerical homogenization.

1. Introduction

The constant increase of computing power coupled with easier-than-ever access to high performance computing platforms enables the computational investigation of materials at the microscopic level: microstructure generation and modeling [1,2], material property prediction and evaluation [3–5], multi-scale analysis [6–9], and within a stochastic framework to include the effects of the input uncertainties at the material level [10]. At the same time, the progress made in the field of material science allows us to control the material microstructure composition to an unprecedented extent [11,12].

Recently, image-based microstructure modeling and analysis have attracted the interest of more and more researchers. One category of research employs voxel-based finite element models using a mesh that is automatically built by converting each voxel into a finite element [13–15]. Given the high computational cost of a voxel-based approach, another theme of research generates image-based microscopic models by incorporating level-sets and the extended finite element method (XFEM) [16,17]. A comparison of the two approaches has been made in a recent work [18]. Thanks to the proposed analysis approaches, the material constitutive behavior can be predicted by imaged-based numerical models. However, access to microstructural images is economically expensive by experiments or time-consuming by numerical simulations [19–21]. Therefore, there is a great demand for an economical and efficient approach to generate microstructure images.

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Techniques of model reduction have been widely used in the fields computational mechanics and multidisciplinary optimization [22,23]. The surrogate models have also been applied in complex structural and shape designs [24–26]. Recently [27,28] used surrogate modeling in structural shape optimization using the coefficient manifolds to reduce the input space. To the knowledge of the authors, the literature reveals little investigation into developing microstructure image generation approach using model reduction techniques. In [29,30], principal component analysis (PCA) has been applied to reduce the parametric space constructed by a large-dimensional data set using the so called *method of snapshots* [31,32]. Each snapshot may be represented as a combination their retained number of eigen-images.

Suppose we have means to generate microstructure representations for instance by varying processing parameters (numerical or experimental, etc.), the goal of this work is to establish a parameterized geometrical description from learning the set of given instances. Using the *method of snapshots*, microstructure snapshots are represented in terms of a POD basis, where the number of modes retained is decided after taking both the image reconstruction errors as well as the convergence of the effective material constitutive behavior obtained by numerical homogenization into consideration. The geometry and topology of individual phases of a parameterized snapshot is given by a series of response surfaces of the projection coefficients using the method of moving least squares (MLS) [33], also called *diffuse approximation* [34]. Two cases are considered:

- When the parameters $\mathbf{v} = [v_1, v_2, \ldots]^T$ of the RVE are known *a priori* as shown in Fig. 1, the parameterized microstructure representation is given by a series of response surfaces of the projection coefficients in terms of $\mathbf{v}$.
- When the parameters are unknown *a priori*, a set of pseudo parameters $\boldsymbol{\eta} = [\eta_1, \eta_2, \ldots]^T$ corresponding to the detected dimensionality of the set of M snapshots (Fig. 1) are locally taken from learning the manifolds of the projection coefficients, and then represent the parametric space using the approximated manifolds with respect to $\boldsymbol{\eta}$.

The ultimate goal of our work is to propose an unified approach for reduced order material representation and behavior; the latter aspect is object of active research [35–37]; in the present article we concentrate on the material representation part of the work. In this paper, the proposed material representation model is applied to numerical homogenization analysis of a set of two-phase composite materials snapshots. The model can also be further applied to analysis such as localized failure in heterogeneous materials [38] and optimal design of the nonlinear behavior of the considered composite [39].

The remainder of this paper is organized in the following manner: Section 2 presents the POD-based interpolation approach for the RVE snapshots. Numerical homogenization in the framework of periodic boundary conditions (PBC) is introduced in Section 3. We showcase the approach and its potential applications by considering a series of two-phase composite RVEs with numerical homogenization in Section 4. The paper ends with concluding comments and suggestions for future work.

2. POD-based RVE interpolation

Without loss of generality, consider a 2D real-valued continuous or discrete material phase indicator function $s = s(x, y, \mathbf{v})$ depending on parameters $\mathbf{v} \in \mathbb{R}^p$, where x and y are the coordinates. Given an $N \times N$ grid of sampling points by the indicator function $[\mathbf{S}(\mathbf{v})]_{ij} = s(x(i), y(j), \mathbf{v})$, $i = 1, \ldots, N, j = 1, \ldots, N$, continuous representation could be discretized giving a representation matrix $\mathbf{S}(\mathbf{v})$, whose precision depends on the resolution, as shown in Fig. 2.

2.1. POD applied to microstructure instances

Consider a set of discrete 2D RVE snapshots $\mathbf{S}_k$ generated corresponding to instances of parameters $\mathbf{v}_k \in \mathbb{R}^P$, $k = 1, \ldots, M$. $\mathbf{S}_k$ is a matrix of dimensionality $N \times N$ attributed with binary values when two-phase microstructures are considered. In order to perform POD reduction, each matrix $\mathbf{S}_k$ is restored in a vector $\mathbf{s}_k$ of length N^2 attributed with real values instead of binary values. By assembling we calculate the deviation and covariance matrices $\mathbf{D}_s$ and $\mathbf{C}_s$:

$$\mathbf{D}_s = [\mathbf{s}_1 - \bar{\mathbf{s}}, \ldots, \mathbf{s}_M - \bar{\mathbf{s}}] \quad \text{and} \quad \mathbf{C}_s = \mathbf{D}_s \mathbf{D}_s^T \tag{1}$$

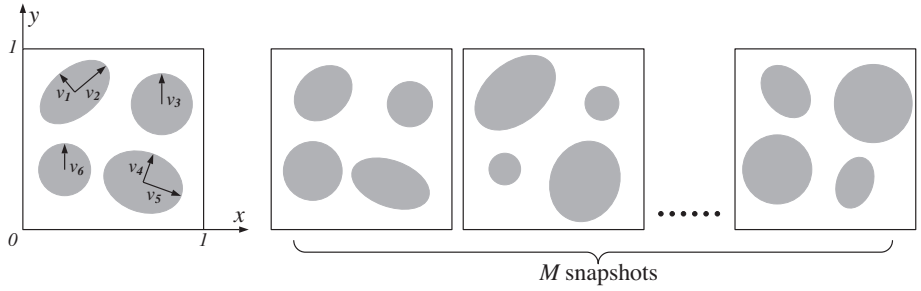

Fig. 1. Illustration of a two-phase, six-parameter microstructure snapshots.