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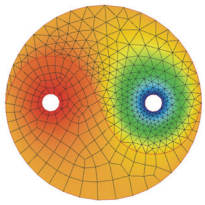

A POD/PGD REDUCTION APPROACH FOR AN EFFICIENT PARAMETERIZATION OF DATA-DRIVEN MATERIAL MICROSTRUCTURE MODELS

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Abstract

The general idea here is to produce a high quality representation of the indicator function of different phases of the material while adequately scaling with the storage requirements for high resolution Digital Material Representation (DMR). To this end, we propose a three-stage reduction algorithm combining Proper Orthogonal Decomposition (POD) and Proper Generalized Decomposition (PGD)- first, each snapshot pixel/voxel matrix is decomposed into a linear combination of tensor products of 1D basis vectors. Next a common basis is determined for the entire set of microstructure snapshots. Finally, the analysis of the dimensionality of the resulting nonlinear space yields the minimal set of parameters needed in order to represent the microstructure with sufficient precision. We showcase this approach by constructing a low-dimensional model of a two-phase composite microstructure.

Key words: parameterization of microstructure, homogenization, voxel approaches, storage costs, material uncertainties

1. INTRODUCTION

The constant increase of computing power coupled with ever-easier access to high-performance computing platforms enable the computational investigation of realistic multi-scale problems. On the other hand, the progress in material science allows us to control the material microstructure composition to an unprecedented extent. In order to accurately predict the performance of structures employing such new materials, it becomes essential to include the effects of the microstructure variation when modeling the structural behavior. The material microstructure varies in a much smaller length scale than the actual structural size. Typical examples include polycrystalline materials, functionally graded materials, porous media, and multiphase polymers. To perform a multi-scale analysis involving these materials, one must first construct models of the microstructure variations to be used as input in the subsequent parameterized analysis. This analysis may be performed in order to answer questions such as: how does microstructure affect the structural behavior? What particular microstructure yields the desired performance? How do the inherent material uncertainties propagate at the structural level?

Given a set of 2D/3D geometrical instances (snapshots) of the Representative Volume Element (RVE) generated from *a priori* known information about feasible microstructure topology, a reduced-order parameterized representation is formulated, which could be directly usable in multi-scale finite element procedures. This problem, similar to those encountered in computer vision image processing and statistical data analysis, requires the right projection space in which the set of snapshots generates

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a low-dimensional manifold that can then be fitted by a parametric hyper-surface.

Basically, the parameterized representation of the material microstructure may be split into two major steps:

1. Low-dimensional model construction of various material properties within the RVE,
2. Using this model as an input to the Finite Element analysis at the RVE level.

The work introduced in this paper utilizes the available sources of information about the variability of the microstructure to construct a set of possible realizations of the material internal structure and mechanical properties. This initial data may be provided by numerical models (Voronoi diagrams, cellular automata,…) or may be experimentally obtained by using imaging techniques: computer tomography (CT), magnetic resonance imaging (MRI), etc. (Ghosh & Dimiduk, 2011). This set of instances – called snapshots, is mapped into a low-dimensional continuous space that spans all the admissible variations permitted by the experimental data. By exploring this low-dimensional equivalent surrogate space, one is essentially sampling over the parameterized space of material topology variations that satisfy the (simulated) experimental data. This low-dimensional representation is subsequently used as an input model in the finite element analysis either via a mesh or a voxel-based variant of finite element model at microstructural scale. The major advantage of this approach is a significant reduction in complexity due to the analysis in a low-dimensional space and results in a drastic reduction in the critical memory requirement.

This representation may then be used in FE2-type multi-scale analysis (Feyel, 2003), in continuous optimization procedures (Sigmund & Torquato, 1997) or within a stochastic framework to include the effects of the input uncertainties at the material level in order to understand how they propagate and affect the performance of the structure (Velamur Asokan & Zabaras, 2006).

The literature reveals little investigation into developing parameterized material representations. Ganapathysubramanian and Zabaras (2007) used Principal Component Analysis (PCA) to represent data-driven representation of the property variations of random heterogeneous media. A general framework has been proposed by Raghavan et al. (2010) for POD-based shape representation by separating the space variables and the design variables in the space optimization context. In this paper, an extension of this technique for material microstructures is made by separating the space variables. The overall goal is to linearly scale the storage requirements in order to cope with the ever-increasing resolution of microstructural snapshots.

The paper is organized in the following manner: section 2 presents the general description of the overall problem. POD and PGD-POD approaches are introduced in Section 3 and 4, respectively. Section 5 compares the reconstruction errors obtained in using the two approaches based on the approximation on a defined two-phase periodic microstructure media. The paper ends with concluding comments and suggestions for future work.

2. PROBLEM DESCRIPTION

Consider a material sample defined by a real-valued continuous $N \times N$ or discrete density map $s = s(x, y, \mathbf{v})$ defined over a square, periodic domain $\Omega = [0,1] \times [0,1]$ and depending on a set of (possibly unknown) parameters (design variables) $\mathbf{v} \in \Re^{\mathbf{p}}$. The problem addressed is how to identify a smallest set of design variables given a set of M snapshots (instances, realizations, samples or images) of the microstructure. The snapshots are given by $N \times N$ matrices $\mathbf{S}_k, k = 1 \ldots M$ such that $[\mathbf{S}_k]_{i,j} = s(\mathbf{x}_n(i), \mathbf{y}_n(j), \mathbf{v}_k)$, $i, j = 1 \ldots N$ with $\mathbf{x}_n$, $\mathbf{y}_n$ defining a regular grid of data points.

1. POD MODEL OF THE MICROSTRUCTURE

Consider a set of discrete 2D snapshots $\mathbf{S}_k$, $k = 1 \ldots M$. Each snapshot matrix is stored in a column vector $\mathbf{s}_k$ of length N^2. The full set of snapshots is stored in an $N^2 \times M$ matrix $[\mathbf{s}_1 - \overline{\mathbf{s}} \ldots \mathbf{s}_M - \overline{\mathbf{s}}]$, centered around the mean snapshot $\overline{\mathbf{s}} = \sum_{k=1}^{M} \mathbf{s}_k / M$. The interpolation may be performed using standard 2D finite element shape functions $\varphi(x, y)$.

$$\tilde{s}(x, y, \mathbf{v}_k) = \varphi^T(x, y)\, \mathbf{s}_k \tag{1}$$

The snapshot matrix may be decomposed by Singular Value Decomposition (SVD)

$$[\mathbf{s}_1 - \overline{\mathbf{s}} \ldots \mathbf{s}_M - \overline{\mathbf{s}}] = \mathbf{U}\mathbf{D}\mathbf{V}^T \tag{2}$$

with the $\mathbf{U}$ and $\mathbf{V}$ matrices containing respectively the left and right singular vectors.

Taking a (reasonable) assumption that $M < N^2$, we define a projection basis composed of the first m

left singular vectors $\Phi = [\phi_1 \ldots \phi_m] \equiv \mathbf{U}[1:N;1:m]$. An arbitrary centered snapshot is approached by

$$\tilde{\mathbf{s}}_k = \overline{\mathbf{s}} + \Phi \alpha_k, \quad \alpha_k = \Phi^T (\mathbf{s}_k - \overline{\mathbf{s}}) \tag{3}$$

The relative Frobenius norm of reconstruction error of the whole matrix of snapshots is

$$\varepsilon = \frac{\sum_{k=1}^{M} (\mathbf{s}_k - \tilde{\mathbf{s}}_k)^T (\mathbf{s}_k - \tilde{\mathbf{s}}_k)}{\sum_{k=1}^{M} (\mathbf{s}_k - \overline{\mathbf{s}})^T (\mathbf{s}_k - \overline{\mathbf{s}})} = \frac{\left\| \sum_{i=m+1}^{M} \sigma_i \phi_i \psi_i \right\|_F}{\left\| \sum_{i=1}^{M} \sigma_i \phi_i \psi_i \right\|_F} = \frac{\sum_{i=m+1}^{M} \sigma_i^2}{\sum_{i=1}^{M} \sigma_i^2} \tag{4}$$

so for dropped off modes ϕ_i, $i = m+1,\ldots,M$ the error is given explicitly by the sum of corresponding diagonal entries σ_i of **D**, squared.

It is thus possible to build a mapping giving for each microstructure instance generated by a set of design variables $\mathbf{v} \in \Re^{\mathbf{p}}$, a unique image $\alpha \in \Re^{\mathbf{m}}$. There are however two problems to be solved:

- an arbitrary $\alpha \in \Re^{\mathbf{m}}$ does not necessarily yield an $\mathbf{v} \in \Re^{\mathbf{p}}$,
- the dimension of $\Re^{\mathbf{p}}$ is not a *priori* known.

Both problems are to be addressed here by building a *manifold of admissible microstructures*. This is done locally for a snapshot by analyzing the local dimensionality of the space spanned by the coefficient vectors α_k. The interpolation of coefficients is then formulated as a minimization problem constrained by manifolds of admissible shapes.

Combining the above with the spatial interpolation functions, we express $s = s(x,y,\mathbf{v})$ for an arbitrary value of design variables not belonging to the initial set and at any point in Ω, possibly not on the grid. The bi-level representation allows us to separate the space variables x and y from the design variables **v**. Assuming that the basis vectors, defined at the grid points, are constant and that only the coefficients α_k depend on the design variables, we rewrite equation (1)

$$\tilde{s}(x,y,\mathbf{v}) = \varphi^T(x,y)\left(\overline{\mathbf{s}} + \sum_{i=1}^{m} \phi_i \alpha_i(\mathbf{v})\right) = \overline{s}(x,y) + \sum_{i=1}^{m} \phi_i(x,y)\,\alpha_i(\mathbf{v}) \tag{5}$$

with $\overline{s}(x,y) = \varphi^T(x,y)\overline{\mathbf{s}}$ and $\phi_i(x,y) = \varphi^T(x,y)\phi_i$.

The storage requirements for this approach are $m \times N^2 + m \times M$ which may be a problem when the resolution of the grid increases. This is even more critical when extending the approach to 3D with the storage becoming $m \times N^3 + m \times M$, which is definitely not scalable as for N = 1024 and M = 100 some 800*GB* (considering 8 byte floating point numbers) are necessary for the modes only and for N = 4096 and M = 1000, with ~50*TB* memory which goes well beyond the capacity of current workstations. The second problem concerns the sensitivity of the modes with respect to the order in which matrix terms are rearranged into a vector.

Therefore, there is a clear need for an approach not requiring renumbering of the matrix entries and scaling better with increasing resolution. The proposed algorithm is presented in the next section.

2. "PGD-POD" MICROSTRUCTURAL MODEL WITH SEPARATED SPACE VARIABLES

In the previous section, an interpolation form separating design variables from the space coordinates is proposed. In this section, a further separation is performed to the individual space dimensions x and y. Given an $N \times N$ grid of sampling points and a matrix snapshot of the density map $[\mathbf{S}_k]_{i,j} = s(x_n(i), y_n(j), \mathbf{v}_k), i,j = 1 \ldots N$, the spatial interpolation of $s(x,y,\mathbf{v}_k)$ is

$$\tilde{s}(x,y,\mathbf{v}_k) = \varphi^T(x)\,\mathbf{S}_k\,\varphi(y) \tag{6}$$

by means of the standard 1D finite element shape functions $\varphi(x)$ and $\varphi(y)$.

Instead of rearranging the matrix snapshots $\mathbf{S}_k$ into a column vector $\mathbf{s}_k$ and performing SVD directly on the data set, the idea is to transform each snapshot $\mathbf{S}_k$ to matrix $\mathbf{E}_k$ of reduced dimensions in terms of two separate basis Φ and Ψ.

$$\tilde{\mathbf{S}}_k = \overline{\mathbf{S}} + \Phi \mathbf{E}_k \Psi^T \tag{7}$$

The dimension of $\mathbf{E}_k$ is now $m_x \times m_y$, decided by the dimensions of the two basis: m_x of Φ and m_y of Ψ, the process of basis extraction is given afterwards (equation10-13). For an arbitrary point (x,y) of the snapshot, we can rewrite equation (6)

$$\tilde{s}(x,y,\mathbf{v}_k) = \overline{s}(x,y) + \varphi^T(x)\,\Phi\mathbf{E}_k\Psi^T\varphi(y) = \overline{s}(x,y) + \sum_{i=1}^{m_x}\sum_{j=1}^{m_y} E_{i,j}(\mathbf{v}_k)\phi_i(x)\psi_j(y) \tag{8}$$

where $\overline{s}(x,y) = \varphi^T(x)\overline{\mathbf{S}}\varphi(y)$, $\phi_i(x) = \varphi^T(x)\phi_i$ and $\psi_j(y) = \varphi^T(y)\psi_j$. For arbitrary value of design and

space variables, the continuous model may now be expressed as

$$\tilde{s}(x, y, \mathbf{v}) = \overline{s} + \sum_{i=1}^{m_x} \sum_{j=1}^{m_y} E_{i,j}(\mathbf{v}) \phi_i(x) \psi_j(y) \qquad (9)$$

Such a 1D approximation in each direction thus transforms every $N \times N$ snapshot $\mathbf{S}_k$ into a $m_x \times m_y$ compressed matrix $\mathbf{E}_k$. The process of extraction of the two separate basis Φ and Ψ is introduced in the following. We start by the truncated SVD decomposition of each individual snapshot

$$\mathbf{S}_k - \overline{\mathbf{S}} = \mathbf{U}_k \mathbf{D}_k \mathbf{V}_k^T \qquad (10)$$

where only the first m_k left and right singular vectors corresponding to the first m_k largest singular values are calculated. Next, we arrange all sub-matrices $\mathbf{U}_k[1:N;1:m_k]$ and $\mathbf{V}_k[1:N;1:m_k]$ into two $N \times (m_1 + \ldots + m_M)$ matrices

$$\mathbf{U}^* = [\mathbf{U}_1[1:N;1:m_1] \ldots \mathbf{U}_M[1:N;1:m_M]] \text{ and}$$
$$\mathbf{V}^* = [\mathbf{V}_1[1:N;1:m_1] \ldots \mathbf{V}_M[1:N;1:m_M]] \qquad (11)$$

and we apply SVD separately to $\mathbf{U}^*$ and $\mathbf{V}^*$

$$\mathbf{U}^* = \mathbf{U}_U \mathbf{D}_U \mathbf{V}_U^T \text{ and } \mathbf{V}^* = \mathbf{U}_V \mathbf{D}_V \mathbf{V}_V^T \qquad (12)$$

The two separate basis Φ and Ψ are composed of the first m_x and m_y left singular vectors from $\mathbf{U}_U$ and from $\mathbf{U}_V$, respectively.

$$\Phi = [\phi_1 \ldots \phi_{m_x}] \equiv \mathbf{U}_U[1:N;1:m_x] \text{ and}$$
$$\Psi = [\psi_1 \ldots \psi_{m_y}] \equiv \mathbf{U}_V[1:N;1:m_y] \qquad (13)$$

Thereafter, the matrices $\mathbf{U}_k$ and $\mathbf{V}_k$ in equation (10) may be now be approximated in terms of the two separate basis Φ and Ψ

$$\tilde{\mathbf{U}}_k \approx \Phi \mathbf{A}_k, \mathbf{A}_k = \Phi^T \mathbf{U}_k \text{ and } \tilde{\mathbf{V}}_k \approx \Psi \mathbf{B}_k, \mathbf{B}_k = \Psi^T \mathbf{V}_k \qquad (14)$$

Substitute above into equation (10) and we have equation (7) where matrix $\mathbf{E}_k = \mathbf{A}_k \mathbf{D}_k \mathbf{B}_k^T$ is the only term depending on the design variables. Once $\mathbf{E}_k$ are obtained, a similar approximation approach is followed to that in section 3. Transforming $\mathbf{E}_k$ to column vector $\mathbf{e}_k$ of length $m_x \times m_y$, SVD reduction is performed on a full set $m_x \times m_y \times M$ matrix $[\mathbf{e}_1 \ldots \mathbf{e}_M]$. Then a new mapping connection is built between each microstructure $\mathbf{v} \in \Re^p$ and the coefficients $\alpha \in \Re^m$ calculated by SVD on $[\mathbf{e}_1 \ldots \mathbf{e}_M]$. The storage requirements for this approach are $(m_x + m_y) \times N + m \times m_x \times m_y + m \times M$ which is significantly less than $m \times N^2 + m \times M$. When extending this approach into 3D, the storage requirement would decrease drastically from $m \times N^3 + m \times M$ to $(m_x + m_y + m_z) \times N + m \times m_x \times m_y \times m_z + m \times M$.

The reconstruction error of all snapshots in this approach is calculated in a similar way as in equation (4). Note that, two factors, m_x and m_y in the basis extraction and m in SVD reduction of $[\mathbf{e}_1 \ldots \mathbf{e}_M]$, actually influence the reconstruction error in this approach.

5. PARAMETERIZATION OF A TWO-PHASE RVE

In this section, a comparison is given for both proposed approaches on a commonly analyzed periodic two-phase microstructure pattern as shown in figure 1. Snapshots of such a pattern could be utilized to model various types of materials and we have a list of them in table 1. The periodic snapshot is defined by two parameters controlling the radii of two groups of circular inclusions. 500 snapshots of resolution 256×256 are randomly generated for a local approximation.

Table 1. *List of possible material types.*

Material Type	Reference
Porous Aluminum	Kouznetsova et al. 2001
Reinforced Alloys	Ghosh et al. 2001
Fiber Composites	Zeman and Sejnoha 2001
Quasi-brittle Materials	Nguyen et al. 2010

Fig. 1. *Two-phase, two-parameter microstructure snapshots.*

5.1. POD approach

SVD is performed directly on the data set. From figure 2, it can be seen that the α's form a set of two-dimensional manifolds rather than a cloud of points in 3D space regardless of the particular triplet of modes used, clearly indicating that the design domain is parameterized by two parameters t_1, t_2, as is known in priori. This means that $\alpha_1 = \alpha_1(t_1, t_2)$, $\alpha_2 = \alpha_2(t_1, t_2)$.... The surfaces formed by α's could be interpreted as the set of all possible "constraints" (direct geometric constraints, technological con-

straints, etc., that are difficult to be expressed mathematically). Therefore, new microstructure snapshot could be generated parametrically in a reduced dimension by taking the surface coordinates t_1 and t_2 as design variables.

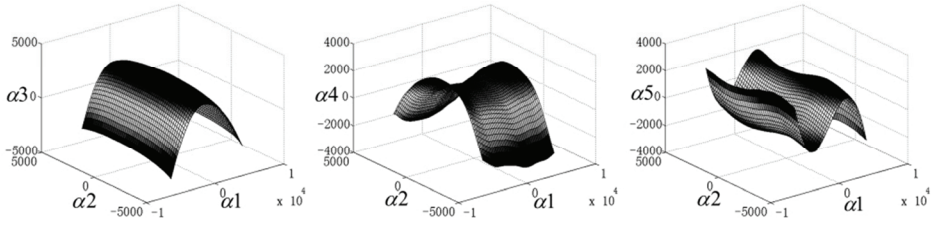

Fig. 2. *2D α-Manifolds for the data set.*

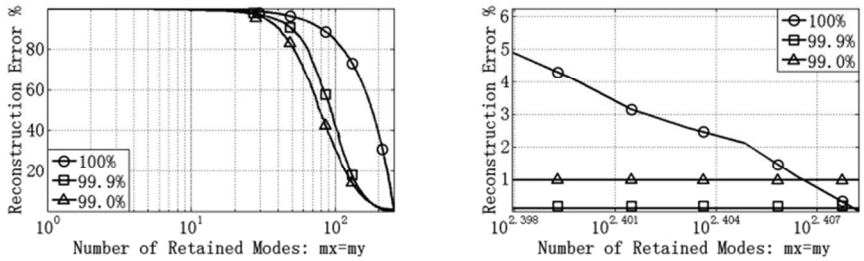

Fig. 3. *Reconstruction errors versus* $m_x = m_y$ *in three cases.*

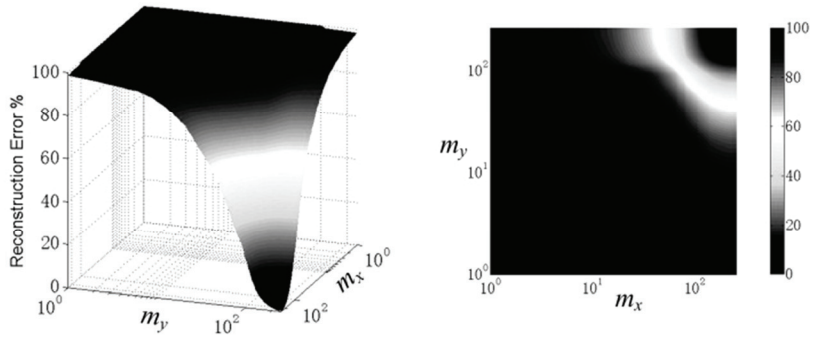

Fig. 4. *Reconstruction errors versus* m_x *and* m_y *in case of square marked curve in figure 3.*

5.2. PGD-POD approach

By extracting basis vectors in both directions, each snapshot matrix **S** is firstly transformed to reduced matrix **E**. For clearer visualization of the reconstruction error in the basis extraction process, we assume $m_x = m_y$ and the errors versus m_x and m_y are given in figure 3. Three curves correspond to cases that different number of modes are retained after the SVD on each snapshot. The curve with data points marked using circles gives the error when retaining 100% projection energy, i.e., $m_1 = m_2 = \ldots = m_M = 256$. The curve with the data points marked using squares is the result of retaining 99.9% projection energy and the average number of retained modes is about 147. When 99% projection energy is retained, the average number of modes is reduced to 122. Such a reduction makes the SVD in equation (13) and (14) a little bit more effective as shown in the curve marked with triangles, but an original error of 1% is introduced at the same time (when $m_x = m_y = 256$).

Note that, m_x doesn't have to equal m_y, especially when anisotropic materials are considered and obviously, the RVE considered here is anisotropic. Figure 4 shows the reconstruction error versus m_x and m_y chosen independently. This means that a further reduction in storage requirement may be achieved by choosing m_x and m_y independently.

Only the case retaining 99.9% projection error is considered for each snapshot SVD. By setting $m_x = m_y = 180$, the data set of 256×256 matrices **S**'s is transformed to reduced 180×180 matrices **E**'s with an introduced error of 4%.

In the next step, POD is performed on the reduced data set of **E**'s. The dimension of the data set is reduced from $256^2 \times 500$ to $180^2 \times 500$. The manifolds formed by the β's (see figure 5) is similar to that in the previous approach, which indicates the microstructure has two parameters and also manifests the fact that PGD maintains the interrelationship among snapshots. The microstructure can be parameterized again by taking surface coordinates t_1 and t_2 as design variables, now within a reduced storage requirement.

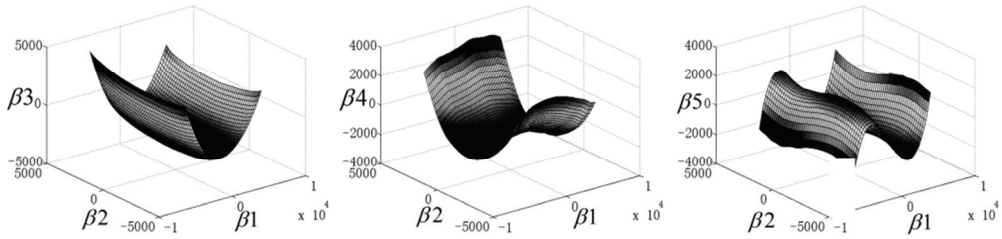

Fig. 5. 2D β-Manifolds for the reduced data set.

5.3. Comparison of the reconstruction errors

A comparison of the reconstruction errors obtained using the two approaches is given in this section. Figure 6 plots the two error curves against the number of retained modes in both approaches. The curve marked with squares, error in POD approach, is calculated by equation (4). The curve marked with triangles, error in PGD-POD approach, is calculated similarly with a presupposition of retaining $m_x = m_y = 180$ in the PGD process.

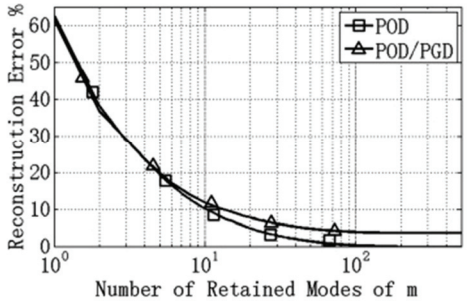

Fig. 6. The reconstruction errors of the two approaches.

Fig. 7. Comparison of the reconstructed snapshots, from left to right: Original Snapshot, POD reconstructed and PGD-POD reconstructed.

Figure 6 shows that the two curves match each other, varying in a similar trend except for the red curve converging to zero while the blue curve converges to a value of 4% due to the reduction in the PGD process. If the expected reconstruction error is no less than 10%, then the numbers of modes needed for the two approaches are close to each other. Considering an error of 20%, we retain the first 5 modes for both approaches. The result of the reconstruction is shown in figure 7, where there is no obvious difference between the two reconstructed snapshots. Thereafter, the PGD-POD approach could achieve a similar result in a much less storage requirement compared to POD approach.

6. CONCLUSIONS AND PERSPECTIVES

A three-stage model reduction scheme combining Proper Orthogonal Decomposition (POD) and Proper Generalized Decomposition (PGD) has been developed to build a reduced order model for the efficient parameterization of material microstructures. The proposed model maintains the high quality of the reconstructed microstructure snapshots with a significantly reduced storage requirement compared to the traditional POD model. With a reduced order model of this type, additional investigations may be conducted into the prediction and optimization of material properties using microstructures.

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PARAMETRYZACJA CYFROWEJ REPREZENTACJI MIKROSTRUKTURY MATERIAŁU POPRZEZ REDUKCJĘ POD/PGD

Streszczenie

Ogólna idea pracy polega na automatycznej generacji precyzyjnej funkcji reprezentującej topologię i geometrię poszczególnych faz materiału celem uzyskania modelu obliczeniowego o minimalnej liczbie parametrów. W tym celu proponujemy trzystopniowy algorytm redukcji obrazu, łączący cechy dekompozycji POD i PGD. W pierwszym etapie, macierz obrazu reprezentatywnego elementu objętościowego jest rozłożona na liniową kombinację tensorowych produktów jednowymiarowych wektorów bazowych. Następnie budujemy wspólną bazę dla całego zbioru obrazów mikrostruktury. W trzecim etapie, analiza wymiaru otrzymanej rozmaitości topologicznej daje minimalny zestaw parametrów potrzebnych do reprezentowania mikrostruktury z odpowiednią dokładnością. Jako przykład podajemy budowę niskowymiarowego modelu dwufazowej mikrostruktury kompozytu.

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