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Deep learning approaches for mining structure-property linkages in high contrast composites from simulation datasets

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ABSTRACT

Data-driven methods are emerging as an important toolset in the studies of multiscale, multiphysics, materials phenomena. More specifically, data mining and machine learning methods offer an efficient toolset for extracting and curating the important correlations controlling these multiscale materials phenomena in high-value reduced-order forms called process-structure-property (PSP) linkages. Traditional machine learning methods usually depend on intensive feature engineering, and have enjoyed some success in establishing the desired PSP linkages. In contrast, deep learning approaches provide a feature-engineering-free framework with high learning capability. In this work, a deep learning approach is designed and implemented to model an elastic homogenization structure-property linkage in a high contrast composite material system. More specifically, the proposed deep learning model is employed to capture the nonlinear mapping between the three-dimensional material microstructure and its macroscale (effective) stiffness. It is demonstrated that this end-to-end framework can predict the effective stiffness of high contrast elastic composites with a wide of range of microstructures, while exhibiting high accuracy and low computational cost for new evaluations.

1. Introduction

An important mission of the field of materials science is to design new/improved materials that can meet the stringent demands placed by emerging advanced technologies. The paradigm of process-structure-property (PSP) linkages plays a central role in capturing and curating the high value materials knowledge needed in this pursuit[1–11]. The extraction and deployment of these linkages has been hindered by the high dimensional representations needed for a rigorous description of the inherently heterogeneous material structure spanning multiple length or internal structure scales. Indeed, the precise physics-based connections between the material structure and its associated properties are very complex. However, from a practical viewpoint of materials design, it is imperative that we capture the high value information in these complex linkages in forms that allow computationally efficient explorations of the extremely large design spaces. Broadly speaking, PSP linkages can be cast in both directions of scale-bridging: (i) homogenization (going from smaller scales to larger scales) [12–14] and (ii) localization (going from larger scales to smaller scales) [11,15–20]. Our focus here will be on homogenization, i.e., prediction of macroscale elastic properties of a high contrast composite given its microstructure information. Contrast in this context refers to the differences in the individual properties of the microscale constituents present in the material microstructure.

The conventional approaches for establishing structure-property linkages in composite materials have relied either on highly sophisticated analytical approaches based on statistical continuum theories [21–23] or on numerical approaches based on finite element (FE) models. Although the statistical continuum theories are very attractive because of their low computational cost (especially significant in exploring large design spaces), progress in this direction has been largely hindered by the need to establish accurately the Green's functions based kernels used in these theories, and the slow convergence of the series expansions for high contrast composites [24,25]. While the numerical approaches such as the finite element models circumvent these challenges effectively, they are not best suited for design explorations of the potentially very large materials space (i.e., solving inverse problems identifying the specific microstructures meeting a designer specified set

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of desired property combinations [4,26,27]).

In recent years, data-driven approaches have attracted the attention of materials science researchers [28–35]. A new framework called Materials Knowledge Systems (MKS) [9,7,15,16,18,36,37] was formulated to take advantage of the relative merits of both the analytical and the numerical approaches described above in formulating structure-property linkages. In this data-driven approach, one first aggregates a sufficiently large ensemble of data points using the numerical approaches, where each data point includes information on the material microstructure (treated as input) and its effective property of interest (treated as output). After establishing the data set, one then calibrates the Green's function based kernels in the statistical continuum theory series expansions to the aggregated data set using suitable regression techniques. This approach has been shown to synergistically combine the respective merits of both the analytical and numerical approaches described earlier, and provide remarkably accurate, low computational cost, structure-property linkages for low to medium contrast composites [7,9,11,15,18,38]. Although the viability of the MKS approach has also been demonstrated for high contrast composites, there continue to be significant hurdles as the application to the high contrast composites requires feature engineering. In this regard, it is noted that feature engineering (i.e., selection of the important microstructure features influencing the effective property of interest) in the context of the MKS framework has been explored mainly using the framework of n-point spatial correlations and principal component analyses [6,37,39–43]. While the current feature engineering approach in the MKS framework was demonstrated to be highly successful in the consideration of the 2-point spatial correlations, its extension to include higher-order spatial correlations is nontrivial. This is mainly because of the explosion in the number of spatial correlations as one goes up systematically to the higher order spatial correlations.

In recent years, deep learning approaches have emerged as the methods of choice in addressing the problem of automated identification of features from an extremely large set of potential features. These methods have enjoyed successes in a broad range of application domains including computer vision (e.g., image segmentation, image classification and face recognition) [44–50]. This emerging new approach significantly outperforms traditional machine learning methods in its ability to learn the embedded model in an aggregated dataset. More specifically, deep learning approaches provide an end-to-end framework where an explicit feature design is not required. Consequently, the trained models usually exhibit higher generalization. Thus, deep learning approaches exhibit tremendous potential for addressing some of the main hurdles in materials research. In [51] Liu et al. applied deep convolutional neural networks to model a large image data collection of polycrastal electron patterns. Liu et al. [52] used deep neural networks to understand the relationship between the composition and the properties of materials. In [53], Li et al. implemented transfer learning approach to reconstruct material microstructures. Cang et al. [54] developed a convolutional deep belief network to automate conversion between microstructure and corresponding lower-dimensional feature representations. Later, Cang et al. [55] applied Variational Auto-Encoder to generate artificial material samples with same morphology distribution as the authentic ones. In [56,57], Yang et al. and Li et al. developed a Generative Adversarial Networks to identify the key microstructure representations and implemented it to design material microstructure with desired properties. Gopalakrishnan et al. [58] applied transfer learning technique to detect crack in pavement.

The target in this study is to establish structure-property linkages for homogenization of high contrast two-phase elastic composites. Homogenization in hierarchical multiscale modeling refers to transfer of information about the microstructure from a lower length scale to higher length scale. This information is usually expressed as an effective property of the material volume being studied and is calculated through various averaging techniques [12–14]. The main challenge in calculating the effective stiffness is to solve the governing field equations formulated at the lower length scale. This is a computationally expensive task if one considers the large space of microstructures that needs to be explored. The proposed deep learning approach will address this task by building data-driven structure-property linkages (i.e., reduced-order models or surrogate models) between the 3-D microstructure and the effective elastic stiffness value.

In this paper, we explore the benefits of using deep learning approaches in establishing high value structure-property homogenization linkages for high-contrast elastic 3-D composite microstructures. In a prior work [59], convolutional neural networks (CNN) were employed to build a model that converts the binary microstructure information into a set of filters that serve as higher-order microstructure information. However, this effort was not strongly explored as a completely feature-engineering free approach. In this study, a standalone CNN is built for the first time to establish structure-property linkages for high contrast elastic 3-D composites using a completely feature-engineering free approach. An extensive analysis of convolutional neural networks with different numbers of convolution and pooling layers was performed. The performance of the CNN is compared to structure-property linkages established with simple physics-based approaches and sophisticated physics-inspired approaches (these will be introduced in Section 3.2) employed in our prior work [7,9,60]. It will be shown through error metrics that CNN built in this study outperforms benchmark methods.

2. Datasets and methods

2.1. Generation of high contrast elastic 3-D datasets

In order to explore and evaluate the performance of CNN models in predicting the effective elastic properties of high contrast composites, we first need to generate a dataset that reflects the ground truth. In this work, because of the lack of a suitable experimental dataset, we assume that the ground truth is reasonably well captured by the results of micromechanical finite element models applied on digitally generated microstructures. Therefore, for this study, we generated 8550 3-D microstructures which are referred to as microscale volume elements (MVEs). The main purpose of these MVEs [7,11,15,18] is to produce the data needed to extract the desired structure-property linkages. They have to be large enough to capture the range of microscale interactions occurring naturally within the microstructural volume element, but small enough to allow for generation and aggregation of the needed data within reasonable computational cost.

The MVEs used in this study were generated by starting with a random assignment of numbers on a uniformly tessellated 3-D spatial (voxelized) grid, following by application of a 3-D Gaussian filter, and finally thresholding to obtain a targeted distribution of volume fractions in the ensemble (i.e., the collection of 8550 MVEs generated for this study). In the effort to generate a rich morphological diversity in the generated set of MVEs, 3-D Gaussian filters with different covariances were employed. The filters were selected in such a way that the MVEs had preferred directionality in three perpendicular directions. Different combinations of diagonal entries in covariance matrix were used to generate MVEs with different amounts of directionality. For this case study, the off-diagonal entries were always kept zero. However, a wider range of diversity in MVEs can be attained by using covariance matrices with non-zero entries in off-diagonal elements as well. Some examples of MVEs with different microstructural details are shown in Fig. 1. The MVE in part (a) is generated by a 3-D Gaussian filter with three identical diagonal entries in the covariance matrix. On the other hand, the microscale constituents of MVEs in part (b), (c) and (d) have clear directionality in x, y and z directions. The degree of directionality of the structural features are controlled with the values of the covariances used with the 3-D Gaussian filters. In total, 57 different 3-D Gaussian filters were employed and each filter is used to generate 150