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Direct microstructure quantification and property prediction of porous materials from X-ray tomography data

Yang Jiao
Materials Science and Engineering, Arizona State University

1. Executive Summary

In this report period, the main focus of the project is to develop quantitative representations of porous materials for efficient material reconstruction, modeling and property prediction, based on limited imaging data. Two approaches have been developed. In the first approach, a variety of lower-order spatial correlation functions, quantitatively characterizing different geometrical and topological features of the materials, are extracted directly from limit x-ray tomographic radiographs. In the second approach, a machine-learning-based generative model has been developed, which implicitly extract salient microstructure features from limited 2D images and generate virtual material microstructures with variable microstructural and physical properties. These developments and the results have been reported in journal publication. The detailed research efforts are summarized below.

2. Quantitative representation of microstructure from limited x-ray tomographic data sets

Accurately quantifying the microstructure of a heterogeneous material is crucial to establishing quantitative structure-property relations for material optimization and design. There is a preponderance of previous work focused on structural quantification based on 2D images and reconstructed 3D volumes obtained via different imaging techniques. We have introduced novel procedures that allow one to extract key structural information in the form of spatial correlation functions from limited x-ray tomography data. In the case where only a very small number of x-ray tomographic radiographs (projections) are available, we derive a formalism based on the Fourier slice theorem to compute angularly averaged correlation functions directly from the radiographs. When a larger number of projections are available, we develop a procedure to extract full vector-based correlation functions. The key component of this procedure is the computation of a "probability map," which provides the probability of an arbitrary point in the material system belonging to a specific phase, via inverse superposition of the scaled attenuation intensities available in the tomography projections. The correlation functions of interest are then computed based on their corresponding probability interpretations from the probability map. The utilities of both of our procedures are demonstrated by obtaining lower-order correlation functions (including both the standard two-point correlation functions and non-standard surface functions) from both parallel-beam (synchrotron) and cone-beam (lab-scale) x-ray tomography projection data sets. Our procedure directly transforms the key morphological information contained in limited x-ray tomography projections to a more efficient, understandable, and usable form.

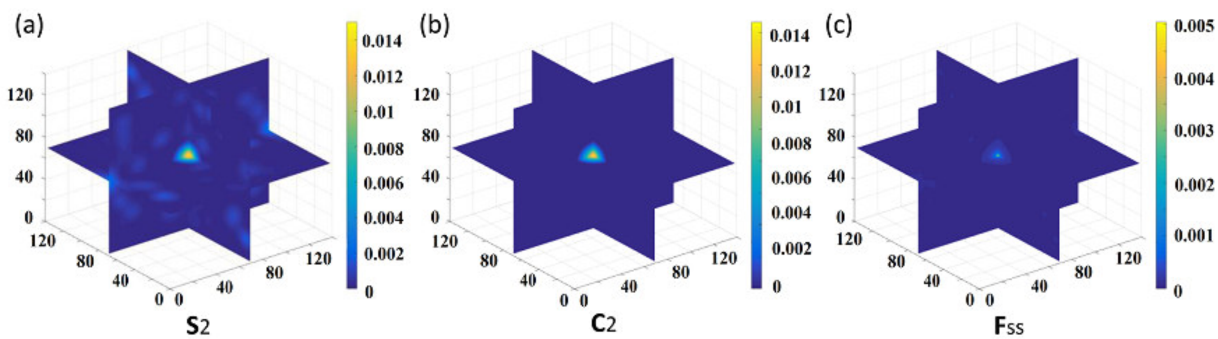

Fig 1: Different types of vector-based lower-order correlation function of a heterogeneous material directly computed from limited tomographic radiographs.

3. Morphology-aware generative model for porous material modeling

Direct prediction of physical properties of a porous material from microstructures through statistical models has shown to be a potential approach to accelerating computational material design with large design spaces. However, statistical modeling of highly nonlinear mappings defined on high-dimensional microstructure spaces is known to be data demanding. Thus, the added value of such predictive models diminishes in common cases where material samples (in forms of 2D or 3D microstructures) become costly to acquire either experimentally or computationally. To this end, we developed a generative machine learning model that creates an arbitrary amount of artificial material samples with negligible computation cost, when trained on only a limited amount of authentic samples. The key contribution of this work is the introduction of a morphology constraint to the training of the generative model, which enforces the resultant artificial material samples to have the same morphology distribution as the authentic ones. We show empirically that the proposed model creates artificial samples that better match with the authentic ones in material property distributions than those generated from a state-of-the art Random Field model, and thus is more effective at improving the prediction performance of a predictive structure-property model.

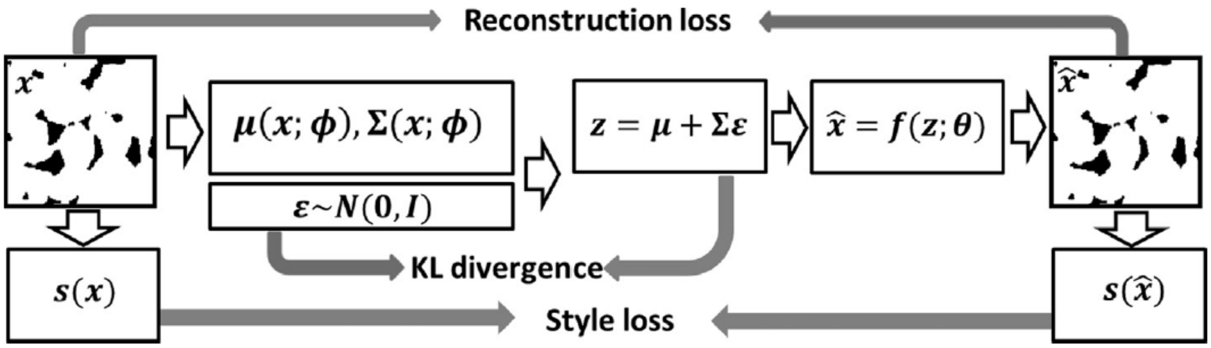

Fig. 2: Schematic illustration of the developed morphology aware generative model for porous material modeling.

4. Impact on PI's career and students participated in the project

The award has allowed the PI to explore novel ideas for developing quantitative microstructure representations for porous materials, directly extractable from limited x-ray tomographic data. The techniques developed using this award can be applied to other heterogeneous material systems with large phase contrast in x-ray absorption, such certain composites and metallic alloys. Novel representations based on a novel set of n-point polytope functions are being investigated, based on which new proposals will be developed to further develop the PI's career.

The student involved in this project has gained experiences in x-ray tomographic imaging, data analysis, effective material property prediction and neural network models, which will significantly benefit the student's future career in R&D or academia. In addition, the student has authored two journal paper reporting results from this project.