Available online at www.eccomasproceedia.org
Eccomas Proceedia UNCECOMP (2025) 357-363

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UNCECOMP 2025
6th ECCOMAS Thematic Conference on
Uncertainty Quantification in Computational Science and Engineering
M. Papadrakakis, V. Papadopoulos, G. Stefanou (eds.)
Rhodes Island, Greece, 15-18 June 2025

A MACHINE LEARNING APPROACH FOR A 2-POINT STATISTICAL HOMOGENIZATION METHOD

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Abstract. *Statistical homogenization methods are widely used to predict the response of a heterogeneous material to loading. A key challenge in applying these methods is the choice of a suitable probability function that accurately captures the material's spatial correlations. However, limitations in both experimental and theoretical tools often lead to difficulties in approximating the statistical descriptor effectively. High computational demands make modelling these complex structures even more complex. To address these challenges, we propose a machine learning based approach to identify a correct correlational descriptor for a class of 2D two-phase-microstructures. A combination of neural networks is used to extract the probability functions from the microstructure image focusing purely on the geometry of the given structure. By coupling a fully connected neural network (FCNN) and a convolutional neural network (CNN), both trained simultaneously, our approach significantly reduces the data requirements, allowing for effective training with a relatively small data set.*

Keywords: Machine Learning, Correlation Functions, Material Modelling, Microstructure Analysis, Data-Driven Neural Network.

ISSN:2623-3339
Peer-review under responsibility of the organizing committee of UNCECOMP 2025.
doi: 10.7712/120225.12361.21109

1 INTRODUCTION

In the fiel of mechanical engineering, there is a wide variety of methods predicting effective material properties under different loading cases such as the multiscale FEM approach [7]. Here, selecting an appropriate representative volume element (RVE) is an essential step, as it provides information necessary for simulating the behavior of a macroscopic body. The connection between length scales is based on the principle of volume averaging and the Hill-Mandel macrohomogeneity condition. The latter ensures the derivation of various boundary conditions for the RVE, thereby establishing a well-posed problem at this level. A closely related problem is the inverse analysis identifying material parameters of nonlinear composites based on the experimental data [6]. Crucial issues here are the investigation of problems involving a large number of unknown material parameters leading to the non-uniqueness of the solution as well as addressing the ill-posedness and determination of the global minimum. In recent years, Machine Learning (ML) techniques have proven to be highly effective in this field A variety of approaches are available, including data-driven and physics-informed neural networks [5, 3], convolutional neural networks (CNNs) [9], and even neural operators [4]. For instance, in [5], an extendable, efficient and explainable ML approach is proposed to model cyclic plasticity and replace conventional material models. This approach combines data-driven and physics-informed network architectures. For statistical homogenization, an explainable statistical represantation on micrstructures using CNNs is presented in [2] . In the present work, we follow a statistical homogenization approach to describe spatial correlation in 2D two-phase microstructures, describing the overall appraoch in section 2. Data and a classical statistical method for correlation function computation are described in section 3, while the Neural Network architecture to replace the process is introduced in section 4, followed by a conclusion and outlook.

2 STATISTICAL HOMOGENIZATION

In materials science, statistical homogenization is a powerful method for predicting the macroscopic response of heterogeneous materials to loading. This approach is particularly useful in cases where materials exhibit complex microstructures, as it enables the derivation of effective properties by considering statistical characteristics of the underlying phases. A crucial aspect of statistical homogenization is the computation of n-point correlation functions. They serve as spatial descriptors of different phases within the material. For two-phase materials, the volume fractions of each phase can be described using 1-point correlation functions.

In this work, we present a neural network architecture designed to predict 2-point correlation functions from microstructure images, addressing a key challenge for statistical homogenization methods in computational materials science. Statistical methods are widely employed to predict material behavior because of their ability to capture the underlying patterns within heterogeneous materials [1, 8]. In their undeformed state, most heterogeneous materials can be effectively described using 2-point correlation functions [10]. For elastic materials, particularly those exhibiting linear elastic behavior, 2-point correlation functions are generally sufficient as the small deformations involved do not significantl alter the material structure. Usually, we are interested in the effective elasticity tensor $\mathbf{C}$, which, in the statistically homogenized version of the local elasticity tensor $\mathbf{c}$, can be written as follows:

$$\mathbf{C} = \langle \mathbf{c} \rangle - \mathbf{G} * \mathbf{F}, \tag{1}$$

with $\mathbf{G}$ denoting the Green's function tensor and tensor $\mathbf{F}$ having components of the form

$$f(\mathrm{r}' \in h_i | \mathrm{r} \in h_j), \tag{2}$$

denoting the probability of r' being in phase h_i under the condition of r being a point within phase h_j. The functions in 2 are called 2-point correlation functions.

3 DATA AVAILABILITY

In data-driven machine learning, the quality and quantity of training and test data sets affect the accuracy and stability of ML-method. Since data availability is scarce, the usage of synthetic data sets is a popular option. Trained on a high quality, big enough dataset, Neural Networks (NN) have high perfomance rates and accuracy. Here, the input data are images of isotropic two-phase microstructure and the outputs are corresponding 2-point correlation functions, which serve as spatial descriptors, quantifying the probability of findin material points in a specifi phase. In 2-isotropic-phase composites, there are four 2-point functions describing the spatial correlation of material phases. A standard way to extract a correlation function descriptor from a microstructure image is the usage of the Monte Carlo method. Since the microstructures under consideration are isotropic, the correlation functions depend only on the distance between two points. Therefore, for a given distance r, one can randomly select two distinct points within the microstructure and count the occurrences of each of the four possible cases, yielding the probabilities $P_{ij}(\mathrm{r})$. In statistically homogeneous media, 2-point correlation functions depend only on the relative position of the two points, making them translationally invariant. To compute these functions, we randomly select 400 points within the microstructure and, for each, evaluate 200 evenly distributed distances in a counterclockwise direction. At each step, we determine whether the sampled point belongs to phase 1 or phase 2 and update the corresponding counters accordingly. This stochastic approach provides an estimation of the desired 2-point probability functions. This generates a statistical Monte Carlo process. For the case of 2- and 3-point probability functions, the process is illustrated in figur 3.

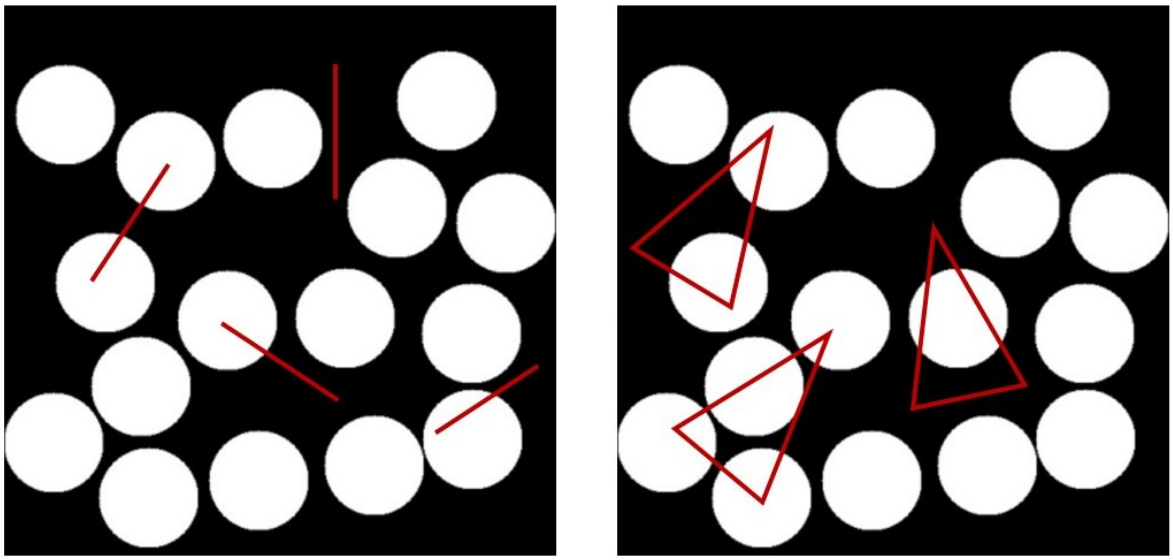

Figure 1: Illustration of the statistical process extracting 2- and 3-point correlation functions, respectively.

For 2-point statistics, the left hand side image shows the randomly placed distance troughout the structure in as red lines, whereas the equivalent process for 3-point statistics requires the traction of points which can be realized by considering triangular shapes and counting the occurence of points in phases at corners of the triangles. In order to generate enough data for the training of a network, we abstract the overall properties of 2D isotropic two-phase microstructures resulting in sqaured black and white images with one phase being black and the other phase being white. The desired material behavior is exhibited by circular inclusions, randomly distributed throughout the material matrix, making this a reasonable choice for synthetic data in ML tasks.

4 ML SURROGATE OF CORRELATION FUNCTIONS

The usage of NNs as a substitute of analytic correlation functions in statistical approaches is a promising research fiel since ML techniques proved to be computationally efficien for many engineering tasks. The four 2-point functions describing the spatial correlation of material phases arising in isotropic two-phase materials are usually extracted by a statistical process like the Monte Carlo method described above. However, this approach is computationally expensive. For this reason, we suggest a solution coupling Convolution Neural Networks (CNN) and Fully Connected Neural Networks (FCNN). Convolutional Neural Networks (CNNs) have emerged as one of the most powerful tools for processing grid-structured data, such as microstructure images. CNNs are a reliable tool in a wide range of applications, including image classification object detection, style transfer (e.g., learning the artistic style of a painter and transforming another image to match that style), image reconstruction, and more. A CNN works by applying a variety of filter to the image and carrying out multiple convolution operations. Mathematically, the convolution operation applied to a 2D $N \times N$-image can be expressed as follows:

$$y(i,j) = f(\sum_{k,l} \mathbf{x}(k,l) \cdot \mathbf{w}(i-k, j-l) + b), \tag{3}$$

with $\mathbf{x}$ the input image, $\mathbf{y}$ the output feature map, $\mathbf{w}$ the filte or kernel, and, as above, b the bias and f the activation function. By performing these operations repeatedly, the network condenses the pixel-level details into a set of higher-level, abstracted representations. This not only reduces data complexity but also highlights the most critical features necessary for subsequent analysis or prediction tasks. Fully connected neural networks (FCNNs) form another fundamental component of deep learning. Once trained on a sufficientl large and diverse dataset, an FCNN becomes a highly efficien and data-driven predictor, capable of rapidly estimating the desired properties of previously unseen data. We suggest a neural network architecture designed to take a microstructure image as input and produce the corresponding 2-point correlation function as output as shown in figur 2. This architecture integrates convolutional and fully connected layers, effectively addressing the unique characteristics of image data and functional data.

Here, unlike traditional tasks where a single function is learned, we deal with an entire class of functions, each exhibiting unique characteristics. Some of these functions are strictly monotonic, while others display non-monotonic behavior with local minima and maxima, which is a key challenge in the determination of an appropriate surrogate. We overcome this problem by combining a CNN and FCNN to simultaneously process both image and functional data. Finally, once both networks have processed their respective inputs, the outputs are merged to create a unifie representation. Employing this multi-path approach, the network is capable of

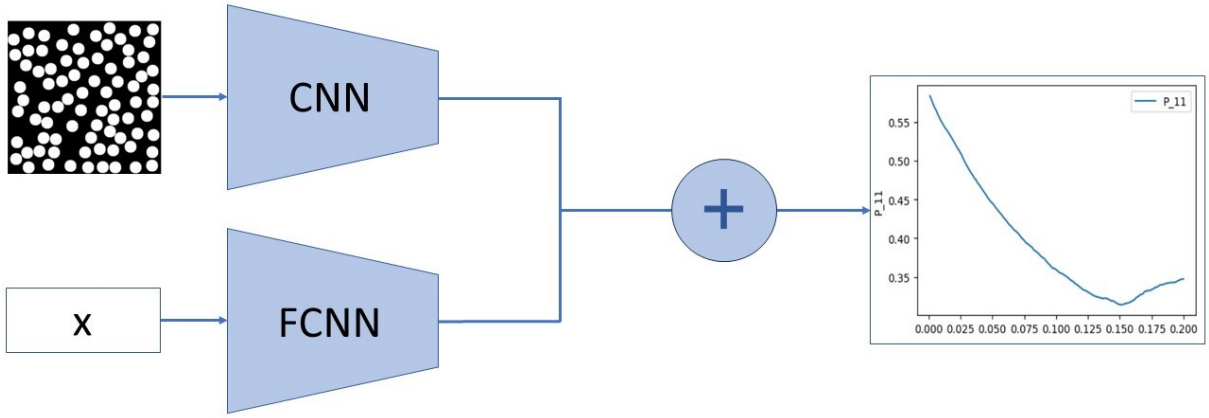

Figure 2: Neural network architecture.

effectively learning a diverse class of functions while maintaining computational efficien y and required accuracy.

The present study considers a range of composites with the inclusion volume fractions of 35-45%. However, the approach is easily adaptable to different ranges of inclusions via extensions in the training data set. Illustrative examples dealing with different microstructures and corresponding correlation functions are shown in figure 3 and 4. In figur 3, the left microstructurehas 60% circular inclusions smaller in size compared to the 57% circular inclusions in the right hand side microstructure image. Due to the bigger size, there are fewer inclusions in the second one. The effect, inclusion sizes have on the monotonocity of the corresponding correlation function, is shown in figur 4. Smaller more scattered second phase inclusion result in a prominentminimum, followd by a local maximum, before the funtion converges to a limit. Our most recent investigation makes use of neural operators to take into account the infinit dimensional nature of the output space as an alternative of CNN-FCNN combination.

5 CONCLUSION AND OUTLOOK

In this work, we successfully developed a neural network architecture capable of predicting 2-point correlation functions for isotropic two-phase materials, specificall for cases with larger inclusion sizes. We achieved accurate predictions even with a relatively small training dataset, demonstrating the network's ability to generalize effectively. Despite these promising results, certain challenges remain. One limitation remaining is the network's performance on micrographs containing smaller inclusions, where the model may struggle to capture fine structural details. Additionally, expanding the variety of microstrcutres, e. g. in terms of the volume fraction range, the network can accurately predict is planned for future work.

To address these challenges, we follow multiple strategies. One approach involves diversifying the training dataset by incorporatinga broader range of inclusion sizes and volume fractions, ensuring that the model is exposed to a more comprehensive set of material structures. Another aspect of current work is refinin the network architecture itself, by introducing modification that enhance its ability to capture fine details or improve its robustness across different material configurations Both of these strategies are currently worked on by the authors.

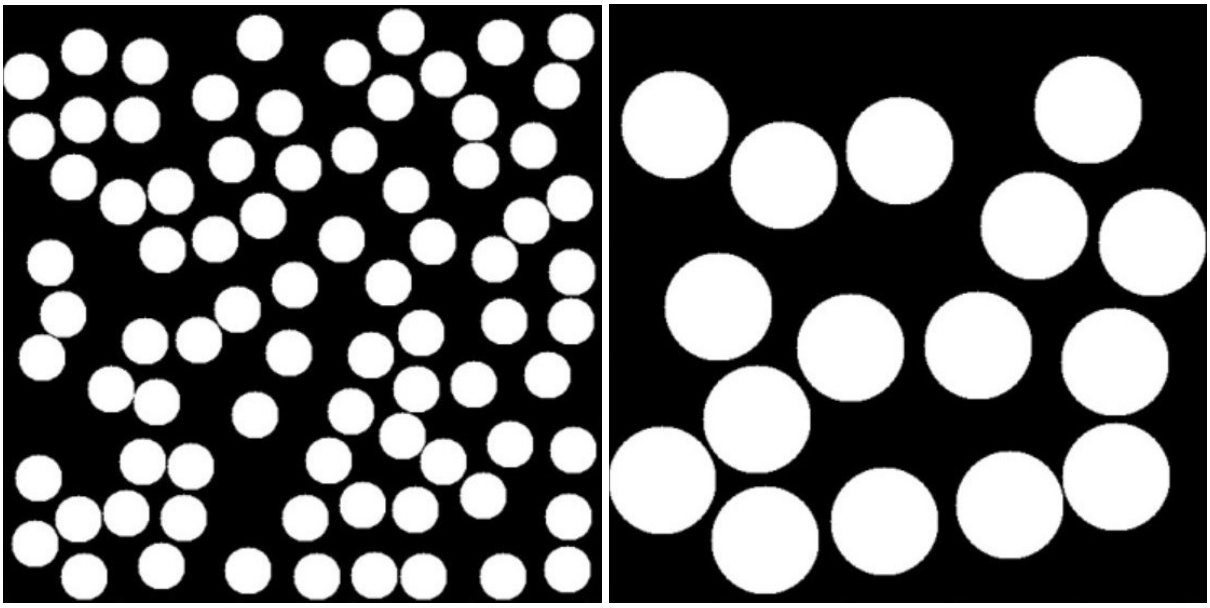

Figure 3: Microstructure image examples.

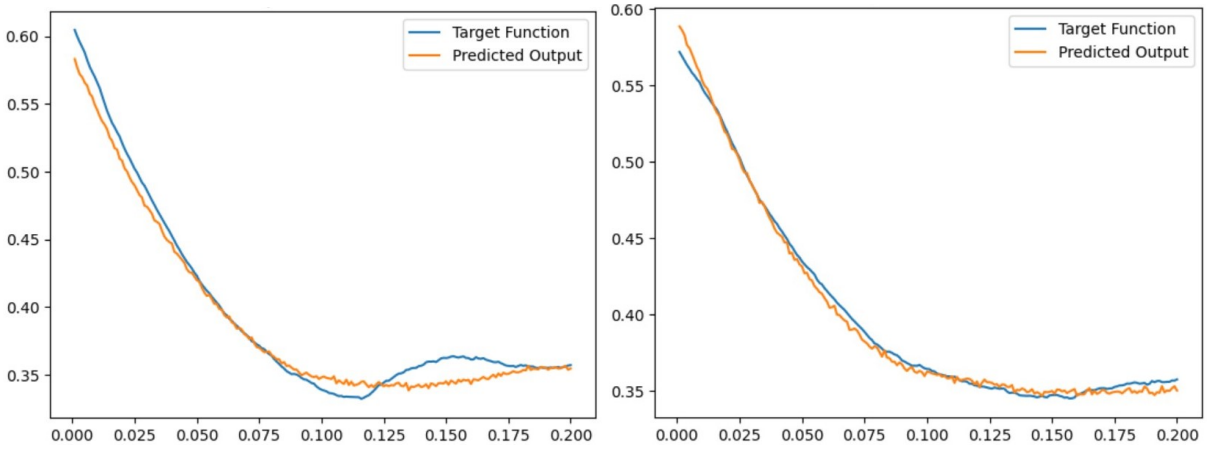

Figure 4: 2-point correlation functions corresponding to the microstructures shown in figur 3.

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