A Multifeatured Data-Driven Homogenization for Heterogeneous Elastic Solids

Ehsan Motevali Haghighi and Seonhong Na *

Abstract: A computational homogenization of heterogeneous solids is presented based on the data-driven approach for both linear and nonlinear elastic responses. Within the Double-Scale Finite Element Method (FE2) framework, a data-driven model is proposed to substitute the micro-level Finite Element (FE) simulations to reduce computational costs in multiscale simulations. The heterogeneity of porous solids at the micro-level is considered in various material properties and geometrical attributes. For material properties, elastic constants, which are Lame’s coefficients, are subjected to be heterogeneous in the linear elastic responses. For geometrical features, different numbers, sizes, and locations of voids are considered to reflect the heterogeneity of porous solids. A database for homogenized microstructural responses is constructed from a series of micro-level FE simulations, and machine learning is used to train and test our proposed model. In particular, four geometrical descriptors are designed, based on N-probability and lineal-path functions, to clearly reflect the geometrical heterogeneity of various microstructures. This study indicates that a simple deep neural networks model can capture diverse microstructural heterogeneous responses well when given proper input sources, including the geometrical descriptors, are considered to establish a computational data-driven homogenization scheme.

Keywords: double-scale FEM; deep learning; multiscale modeling; homogenization; elasticity; heterogeneity

1. Introduction

Heterogeneity is one of the essential characteristics of natural materials, including soils and rocks. The heterogeneous structures of a natural system can be well represented at a specific scale. In most cases, these features can be identified along with different scales. Depending on the size of interest, a hierarchical system of heterogeneity may be found that spans multiple scale levels. In terms of the modeling aspect, bridging different scales without losing the information of heterogeneity is a challenging task. Obviously, it is impossible to consider all the heterogeneous structures of materials along with different scales explicitly. Therefore, a material as a two-scale or three-scale system is idealized to account for various heterogeneous features through constitutive laws or multiscale simulations (e.g., Feyel and Chaboche [1], Liu et al. [2], Wang and Sun [3], Na and Sun [4]).

The concurrent multiscale method associated with homogenization theories is known as a powerful approach to analyzing the hierarchical system of materials. In particular, computational homogenization is one of the most popular approaches to systematically incorporating material and geometrical heterogeneities. Please refer to more details about the computational homogenization with relevant techniques and assumptions [5]. In the Finite Element Method (FEM) context, the double scale finite element (FE2) method can be used for multiscale simulations to incorporate microscopic heterogeneity into a macroscopic problem (cf. Feyel [6]). The microscopic heterogeneity is presented by the representative volume element (RVE), which has a sufficiently large size to effectively include all microscopic heterogeneities that occur in the material [7]. Since each integration
point of the macroscopic FE model associates with the microscopic FE simulation, the FE\(^2\) technique requires a significant amount of computational cost in general. Thus, reducing this computational complexity in multiscale methods is one of the most critical issues to efficiently and systematically investigating heterogeneous materials.

There are many studies to reduce the computational complexity and cost systematically. As an example, the Proper Orthogonal Decomposition (POD) method extracts a group of orthogonal bases of a system to approximately represent the system with the reduced degree of freedom, which decreases the complexity of the problem [8]. This approach has further extended to signal analysis and pattern recognition [9], as well as fluid dynamics and coherent structural problems [10]. Another example is Transformation Field Analysis (TFA), which reduces the number of the internal variables by assuming the microscopic field of the internal variable to be piecewise uniform [11]. The TFA is applied to the more complex behaviors such as thermo-viscoelasticity or damage [12]. Using the image of microstructures, the local and overall responses of the material can be captured using Fourier Transform-Fast Fourier Transform Homogenization (FFTH), which is to find a homogenized behavior within the heterogeneity of microstructure [13]. In addition, a strain energy equivalent based RVE is developed, assuming mechanical equivalence of micro and macro levels, to simulate the prefabricated composite slab [14,15].

One innovative idea for reducing the complexity of the multiscale heterogeneous system is incorporating Artificial Intelligence (AI) methods. The expression of “Artificial Intelligence” was firstly coined by McCarthy [16], which can be defined as the ability of machines to think differently than humans [17]. Most of the early works used AI methods to capture the mechanical constitutive behavior of materials directly. For example, one of the pioneering attempts was presented by Ghaboussi et al. [18], which predicted the plane stress behavior of concrete in both uniaxial and biaxial conditions using the neural network. Later, Ghaboussi et al. [19] developed an autoregressive model to capture the load-deflection behavior of materials. The recurrent neural network was first utilized for training the mechanical behavior of materials [20], in which the water pressure associated with strain and porosity was adopted as inputs. Huber and Tsakmakis [21] considered material properties as features for training the neural network, and then they predicted a load-deflection behavior. Similarly, Pernot and Lamarque [22] used the neural network to learn constitutive laws; they used \(\sigma_{xx}\) and \(\sigma_{zz}\) aligned with porosity and friction angle for the prediction of soil behavior.

AI methods have also been used for homogenization in the multiscale aspects to reduce computational calculations. In 2001, Haj-Ali et al. [23] developed a pre-trained material model based on Artificial Neural Network (ANN) to capture the nonlinear and damage behavior of heterogeneous materials. This approach utilized the strain, geometry, and damage information as input and the stress as output for training the micromechanical behavior. Recently, Mozaffar et al. [24] trained path-dependent behavior of a material using a stacked long-short term memory unit (LSTM) for the first time. They predicted the total stress tensor provided the full strain tensor, which is beneficial for concurrent multiscale methods. Ali et al. [25] applied a machine learning method for plastic polycrystals by introducing descriptors that represent the geometry of microstructures. In contrast, unsupervised machine learning was also used for path-dependent behaviors. For example, Wang et al. [26] developed a cooperative game for the automated learning of elastoplastic material responses. Regarding FE\(^2\) scheme, Ghavamian and Simone [27] developed a data-driven model for path-dependent materials using the LSTM, where the consistent tangent was calculated using the auto-differentiation of TensorFlow. Similarly, Capuano and Rimoli [28] leveraged surrogate modeling to reduce the computational cost by establishing a direct relationship between the inputs and outputs of finite elements.

In this study, a computational data-driven homogenization for heterogeneous materials is developed to efficiently incorporate the microscopic features in material and geometrical aspects. Here elastic responses is only considered (linear and nonlinear), and the single-phase system of porous solids is considered to focus on mechanical responses. A
novel numerical experiment is designed to generate a database for micromechanical responses of the heterogeneous solids. The first design of experiment (DOE) includes various microstructures by randomly generating void spaces with different numbers and sizes. The geometrical features of microstructures are coined as descriptors, which are expressed by the probabilistic information of the pore structures. Then, different material properties are considered to account for the material heterogeneity. Diverse micromechanical behaviors are recorded via the homogenization scheme for FE, where the information of mechanical responses, including the strain and both material and geometrical information of microstructures, are considered inputs of the training process. Then, a Deep Neural Network system is established to predict the stress responses finally. The proposed model demonstrates an excellent capability of the homogenization method in capturing the elastic (linear and nonlinear) responses of heterogeneous porous solids.

The organization of this paper is as follows. In Section 2, the double scale finite element method and the Deep Learning method are described to explain the theoretical background of the paper. In Section 3, the design of the experiment for generating data is presented in three aspects: (1) generation of heterogeneous microstructure, (2) extracting microstructural descriptors, and (3) generation of loading path. Section 4 covers two problems to test the designed Deep Neural Network in predicting random and monotonic loading paths followed by Discussion (Section 5). The following notations and symbols are used throughout: bold-face letters denote tensors and vectors; the symbol “·” denotes an inner product of two vectors (e.g., \(a \cdot b = a_i b_i\)), \(\cdot\) or a single contraction of adjacent indices of two tensors (e.g., \(c \cdot d = c_{ij}d_{ij}\)); the symbol “:” denotes an inner product of two second-order tensors (e.g., \(c : d = c_{ij}d_{ij}\)). Following the standard mechanics sign convention, stress is positive in tension and negative in compression.

2. Overview of Methods

In this section, the methods and numerical tools implemented in this study are presented. First, the FE\(^2\) framework is presented, which is used to simulate a dataset consisted of a set of strain and stress. Second, the deep learning and back-propagation algorithm are explained.

2.1. Homogenization Technique

In this section, the multiscale modeling method implemented via the FE\(^2\) associated with the computational homogenization is briefly summarized. Both micro and macro levels are discretized based on the finite element method. In each integration point of the macroscopic FE domain, the microscopic FE simulation is conducted, in which the homogenized microscopic behavior is returned to the macro level. More detailed description can be found in multiple sources (e.g., Miehe and Koch [29], Kouznetsova et al. [30]).

The homogenization technique for the FE\(^2\) framework is presented within the following subsections. It is worth noting that small “m” stands for the micro-level and capital “M” depicts the macro-level. In addition, \(\{u : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}^3\}\) denote the displacement space of the material point \(x \in \mathbb{R}\) and \(\varepsilon := \text{sym} [\nabla u]\) be a microscopic strain on time \(t \in \mathbb{R}\) of the microstructure \(\mathbb{R} \subset \mathbb{R}^3\) [27].

2.1.1. Macro-Level Governing Equation

The following governing equation is used to describe the deformation of the macro-level domain,

\[
\nabla \cdot \sigma_M = 0 \quad \text{in} \quad \Omega_M, \quad (1)
\]

where \(\sigma_M\) is the macro stress, \(\nabla\) is the differential operator, and \(\Omega_M\) is the macro-level space. The boundary conditions \(\Gamma^u_M = \Gamma^u_M + \Gamma^v_M\) (Dirichlet \((\Gamma^u_M)\) and Neumann \((\Gamma^v_M)\), respectively) are applied on the \(\Omega_M\) space. In this study, macro stress is defined as a function of the macro strain connected through the micro-level simulation,

\[
\sigma_M = \mathbb{N}(\varepsilon_M), \quad (2)
\]
where \( \sigma_M \) is the macro stress, \( \varepsilon_M \) is the macro strain, and \( N(\cdot) \) is a function describing the micro-level simulation.

The weak form of the governing equation is derived based on the FEM procedure; thus, at each time step, the discretized weak form can be obtained as,

\[
K_M du = f_M^{\text{ext}} - f_M^{\text{int}}
\]

(3)

where \( K_M = \int_\Omega M^T D_M B_M \sigma_M \), \( f_M^{\text{int}} = \int_\Omega B_M^T \sigma_M \), \( f_M^{\text{ext}} = \int_{\Gamma_{\text{M}}} N_M^T t_M \) are the macro stiffness matrix, macro internal force, and macro external forces, respectively. \( N_M^T \) is the macro-level shape function, \( B_M \) is the derivative of macro-level shape function, and \( D_M \) is the macro consistent tangent stiffness matrix.

To localize the displacement field on the boundary of the representative volume element (RVE), a linear displacement boundary condition is used on the micro-level [29]. Based on this method, the deformation boundary constraints in terms of the macro strain (\( \varepsilon_M \)) can be obtained as,

\[
u(x, t) = \varepsilon_M x \quad \text{at} \quad x \in \partial \vartheta \]

(4)

This condition defines the linear deformation on the boundary of the RVE (\( \vartheta \)). To be specific, at each node \( q \) of the surface boundary of microstructure, one may obtain,

\[
u_q = \varepsilon_M x_q, \quad q = 1, \ldots, M
\]

(5)

where \( \varepsilon_M \) is the macroscopic strain, and \( x_q \) is the boundary node displacement matrix of the RVE. In other words, one can obtain,

\[
\varepsilon_M = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{22} & 2\varepsilon_{12} \end{bmatrix}^T \quad \text{and} \quad \nu_q = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}_q
\]

(6)

For 2D case, it can be demonstrated as,

\[
u_q = D_q^T \varepsilon_M, \quad q = 1, \ldots, M
\]

(7)

where \( D_q \) is a matrix that depends on the coordinate of nodal points in the RVE of microstructures, and it can be obtained as,

\[
D_q^T = \frac{1}{2} \begin{bmatrix} 2x_1 & 0 \\ 0 & 2x_2 \\ x_1 & x_2 \end{bmatrix}_q
\]

(8)

where \( x \) is defined as the displacement at the micro-level.

2.1.2. Micro-Level Equilibrium Equation and Homogenization

At the micro-level, the equilibrium equation can be simply shown as,

\[
\nabla \cdot \sigma_m = 0 \quad \text{in} \quad \Omega_m
\]

(9)

where \( \sigma_m \) is the stress at the micro-level, and \( \Omega_m \) is the volume of the RVE of microstructures. As described in the preceding section, the Dirichlet boundary is applied in the micro-level domain. In this study, the stress–strain relationship at the micro-level is described either by linear or nonlinear elasticity. In the case of linear elasticity, the relationship between stress and strain can be obtained as,

\[
\sigma_m = E : \varepsilon_m
\]

(10)

where \( E \) denotes the rank-four tensor of elastic modulus, which can be given as,

\[
E_{ijkl} = K\delta_{ij}\delta_{kl} + \mu \left( \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl} \right)
\]

(11)
where \( K = \lambda + \frac{2}{3} \mu \), and \( \mu \) and \( \lambda \) are first and second Lame’s coefficients.

For the nonlinear elastic model, the following hypoelastic constitutive law [31] is considered:

\[
\begin{align*}
\sigma_{ij} &= S_{ij} + \sigma_{kk} \frac{\delta_{ij}}{3} \\
S_{ij} &= \frac{2}{3} \sigma_e \epsilon_{eij} \\
\sigma_{kk} &= \frac{E}{1-2\nu} \frac{1}{3} \epsilon_{kk} \\
\epsilon_{ij} &= \epsilon_{ij} - \frac{1}{3} \epsilon_{kk} \delta_{ij} \\
\epsilon_e &= \sqrt{\frac{2}{3}} \epsilon_{ij} \epsilon_{ij} \\
\sigma_e &= \begin{cases} \\
\sqrt{1+\frac{n^2}{(n-1)^2} - \left( \frac{n}{n-1} - \frac{1}{2} \right)^2} & \epsilon_e \leq \epsilon_0 \\
\left( \frac{\epsilon_e}{\epsilon_0} \right)^{\frac{n}{n-1}} & \epsilon_e \geq \epsilon_0 
\end{cases}
\end{align*}
\]

(12)

where \( \sigma_e \) is the micro stress, and \( \epsilon_m \) is the strain at the micro-level. It is worth mentioning that \( E \) and \( \nu \) denote Young’s modulus and Poisson’s ratio, respectively. The nonlinear FEM procedure is employed, which leads to the discretized weak form as,

\[
K_m du = -f^{int}_m
\]

(13)

where \( K_m = \int_{\Omega_m} B_m^T D_m B_m \) and \( f^{int}_m = \int_{\Omega_m} B_m^T \sigma_m \) are the micro stiffness matrix, and micro internal force, respectively. \( B_m \) is the derivative of micro shape function and \( D_m \) is the micro consistent tangent stiffness matrix.

For homogenization of micro-level responses, The nodes should be partitioned into two groups [29]: interior nodes of the RVE, \( x_a \in \mathcal{V} \), and exterior nodes, \( x_b \in \partial \mathcal{V} \) (Note: \( \mathcal{V} \) is the RVE associated with microstructures). Therefore, the internal force vector \( f(u) \) and associated tangent \( K(u) \) of the discretized microstructure can be partitioned as,

\[
f = \begin{bmatrix} f_a \\ f_b \end{bmatrix}, \quad K = \begin{bmatrix} K_{aa} & K_{ab} \\ K_{ba} & K_{bb} \end{bmatrix}
\]

(14)

The homogenized tangent stiffness matrix can be obtained as,

\[
\bar{K}_{bb} = K_{bb} - K_{ba} K_{ab}^{-1} K_{ab}
\]

(15)

\[
\bar{C} = \frac{1}{|\mathcal{V}|} \mathbb{D} \tilde{K}_{bb} \mathbb{D}^T
\]

(16)

where \( \bar{C} \) is the homogenized tangent stiffness. Finally, for the homogenization of stress, we have,

\[
\bar{\sigma} = \frac{1}{|\mathcal{V}|} \mathbb{D}^T f_a
\]

(17)

where \( \mathcal{V} \) is the volume of the RVE of microstructures.

2.2. Deep Learning (DL)

Considering the application of Artificial Intelligence in interpreting and learning human actions, many studies have implemented deep learning to interpret and learn the behavior of microstructure [24]. Since Deep Learning (DL) is robust to find a mapping from input to output, the DL is able to open a new insight for averaging the behavior of microstructure and decreasing the computational complexity of the system by circumventing micro-scale calculations. In this study, a DL method is implemented through a simple neural network to capture the microscopic behavior of the elastic heterogeneous porous
solids. This process is conducted by (1) generation of datasets and (2) development of a data-driven model, in which an offline-based computational homogenization is established for microscopic FE simulations.

Figure 1 depicts a conceptual diagram of a deep neural network (cf. [18]). The structure of a neural network consists of unit neurons or processing units. Every neuron is connected to the other neurons throughout a pathway that has a particular weight multiplied by the incoming signal. The weight of each pathway demonstrates synaptic efficiency. The outgoing signal from the neuron is pathed throughout a binary function called the activation function, which controls the output with a threshold. Based on this structure, each neuron applies a specific threshold and maintains part of the information. With this method, the information propagates to the end of the network, the output. In short, the neural network system consists of several layers called input, hidden, and output layers, where the propagation of information is forwarded from the input to the output layer.

![Deep Neural Network Diagram](image)

**Figure 1.** Conceptual diagram of a Deep Neural Network, the arrow depicts the flow of information through which the synaptic weight is considered.

The learning process, which means finding optimal weights, is performed by the supervised learning method [32]. This process provides the target data from the initial state (Input Layer), and the goal of training is mapping from the input data to target data. At the initial step of the training process, the initial weights are assigned by generating a random number and then given the input data, the information flow toward the output layer. Compared with the obtained output with given target data, the error is calculated then backpropagates from output to input in order to update the weights. The optimization of the weights is calculated throughout the gradient descent method, that may be expressed simply as,

$$\delta w_{ij} = \eta \delta_j O_j$$

where \(\eta\) is the learning rate, and \(\delta_j\) is the gradient of the total error with respect to net input at unit \(j\). The \(\delta_j\) can be computed with the difference between expected \((t_j)\) and computed output \((a_j)\) as,

$$\delta_j = (t_j - a_j) F'(N_j)$$

where \(F'\) is the derivative of the activation function [18].

An activation function of a node in a neural network transforms an input or a summation of weighted inputs to output. The activation function is one of an essential components that decides the level of complexity in prediction by adding nonlinearity. The most well-known nonlinear activation functions are the sigmoid and tanh functions, which are used to map an input into \((0\) and \(1)\) and \((-1\) and \(1)\), respectively. Another widely used activation function is ReLu, which is a piecewise linear function that transforms input to directly
output if it is positive, and otherwise, it will output zero. In this study, ReLu and tanh activation functions are selected [33].

3. Design of Experiment (DOE)

This study aims to reduce the computational complexity and cost of running a large number of microscopic simulations in the FE$^2$, by developing a computational homogenization technique through a data-driven approach based on Artificial Intelligence—Deep Learning. To achieve this goal, series of virtual experiments are designed for the FE$^2$ framework to generate the database of homogenized microscopic behaviors. Since the quality and quantity of datasets for deep learning are essential, the data generation process is established such that the datasets well reflect the microscopic behaviors for a data-driven model. Firstly, the heterogeneity of elastic solids is considered through different numbers and sizes of micro-pore structures. Then, geometrical descriptors are described to represent various microstructures as input. Finally, the loading conditions for the microstructures are presented, which are designed for micro-mechanical behaviors.

3.1. Generation of Microstructures

The homogenized behavior of heterogeneous materials are resulted from both geometrical and material properties. In this study, the geometrical heterogeneity is considered by randomly generated voids of porous microstructures. For the microstructures with various sizes and numbers of voids, properties of the solid domain are also changed to consider the material heterogeneity. The RVE of microstructures is adopted as a square domain, that is, 1.0 by 1.0 m, where only circular voids are considered with the range of radius from 0.05 to 0.2 m. Each void locates inside the RVE domain with the constraint of a full circle. In other words, no voids are overlapped or intersected with the domain boundary.

Based on these conditions, the radius and the center of voids are selected as random variables (using uniformly distributed random number-equal probability over a given range) to generate 100 different microstructures. Figure 2 depicts three samples of randomly generated microstructures. All randomly generated microstructures are labeled with numbers. For generating mesh and geometry, we use pdetool of MATLAB, in which pdemsh function is used by considering a linear three-noded triangle element. The mesh growth rate of 1.5, which is the rate at which the mesh size increases away from the small parts of the geometry, is considered.

![Figure 2](image)

**Figure 2.** Three samples of randomly generated microstructures: The radii and the centers are selected randomly and are limited to prevent them from overlapping with other voids or not to intersect with the domain’s boundary. (a) Microstructure #15, (b) Microstructure #35, and (c) Microstructure #50.

3.2. Extracting Microstructure’s Descriptors

For intelligent homogenization, key characteristics of microstructures should be identified to represent their heterogeneity in the training process. This section describes the unique features that define the geometrical heterogeneity of microstructures, which are referred to as descriptors. To reduce the complexity, we extract four probabilistic descriptors utilizing a low order of information, which reflects the convexity, porosity, and distribution of voids.
3.2.1. N-Point Probability Function

Consider \( x \) as a fixed point, where the domain of our interest consists of two phases: solid and void spaces. An indicator function \( \mathcal{L}^{(i)}(x) \) that has two possible values 0 (phase a) and 1 (phase b) for some realizations \( \theta \) can be defined. In other words, the indicator function, \( \mathcal{L}^{(i)}(x) \), can be considered a binary random variable (cf. [34]). Therefore, the probability of \( \mathcal{L}^{(i)}(x) = 1 \) may be simply expressed as,

\[
P\{ \mathcal{L}^{(i)}(x) = 1 \}.
\]

(20)

Accordingly, the probability of \( \mathcal{L}^{(i)}(x) = 0 \) can be expressed as,

\[
P\{ \mathcal{L}^{(i)}(x) = 1 \} = 1 - P\{ \mathcal{L}^{(i)}(x) = 1 \}.
\]

(21)

Therefore, the expectation value of any function \( \mathbb{E}[\mathcal{L}^{(i)}(x)] \) can be given as,

\[
\mathbb{E}[\mathcal{L}^{(i)}(x)] = P\{ \mathcal{L}^{(i)}(x) = 1 \} \mathbb{E}(1) + P\{ \mathcal{L}^{(i)}(x) = 0 \} \mathbb{E}(0).
\]

(22)

It is noted that angular brackets indicate an ensemble average, that is, an average over all realizations \( \theta \) of the ensemble [34]. Based on this definition, the expectation value of a specific case is further considered when \( \mathbb{E}[\mathcal{L}^{(i)}(x)] = \mathcal{L}^{(i)}(x) \), that is,

\[
S^{(i)}_1(x) \equiv \mathbb{E}[\mathcal{L}^{(i)}(x)] = P\{ \mathcal{L}^{(i)}(x) = 1 \}.
\]

(23)

In other words, the expectation of the indicator function \( \mathcal{L}^{(i)}(x) \) can be obtained directly from the probability \( P\{ \mathcal{L}^{(i)}(x) = 1 \} \). Followed by Torquato and Haslach Jr [34], the \( S^{(i)}_1(x) \) is called the first order (one-point) probability function. To be specific, this one-point probability function, \( S^{(i)}_1(x) \), gives the probability of the phase \( i \) at position \( x \).

Now, all \( x \) in the domain of our microscopic RVE \( V \) is considered. According to the definition of the indicator function, the realization of \( \theta \) in \( V \), that is \( V_i(\theta) \), is the same as \( \mathcal{L}^{(i)}(x, \theta) \) for all \( x \) in \( V \). Therefore, the collection of random variables \( \mathcal{L}^{(i)}(x) \) is consistent with the random set \( V_i(\theta) \). In other words, the probabilistic description of \( V_i(\theta) \) is given by the joint distribution of \( \mathcal{L}^{(i)}(x) \), that is,

\[
\mathcal{L}^{(i)}(x_1)\mathcal{L}^{(i)}(x_2)\cdots\mathcal{L}^{(i)}(x_n) \quad \text{as} \quad n \geq 1,
\]

(24)

where \( x_1, x_2, \ldots, x_n \) changes over \( V \) with the integer \( n \) [34]. Since the \( \mathcal{L}^{(i)}(x) \) is either 0 or 1, the probability of the amount can be specified as,

\[
P\{ \mathcal{L}^{(i)}(x_1) = j_1, \mathcal{L}^{(i)}(x_2) = j_2, \ldots, \mathcal{L}^{(i)}(x_n) = j_n \}
= P\{ \mathcal{L}^{(i)}(x_1) = 1, \mathcal{L}^{(i)}(x_2) = 1, \ldots, \mathcal{L}^{(i)}(x_n) = 1 \},
\]

(25)

where each \( j_n \) is either 0 or 1.

Similar to the one-point probability function, the expectation of the product is considered as, \( \mathcal{L}^{(i)}(x_1)\mathcal{L}^{(i)}(x_2)\cdots\mathcal{L}^{(i)}(x_n) \) as,

\[
S^{(i)}_n(x_1, x_2, \ldots, x_n) \equiv \mathbb{E}[\mathcal{L}^{(i)}(x_1)\mathcal{L}^{(i)}(x_2)\cdots\mathcal{L}^{(i)}(x_n)],
\]

(26)
which can be defined as the n-point probability function for phase $i$ \cite{34}. In other words, this function yields the probability that $n$ points at position $x_1, x_2, \cdots, x_n$ are found in phase $i$.

The N-point probability function is implemented to represent the geometric information of microstructures within a succinct format. Firstly, the 1-point probability function (Figure 3) can be obtained by randomly drawing multiple points on the RVE domain and calculating a fraction of the points that are positioned inside voids. This 1-point probability function yields the porosity of the microstructure. Similarly, the distribution of voids can be represented using the 2-point probability function (Figure 3). For the 2-point probability function, two points are randomly drawn in one trial. Out of multiple casts, we calculate the probability when both two points are outside of any voids. The 3-point probability function (Figure 3) is further utilized to have more in-depth information about the distribution of voids. Again, the probability can be determined when all 3 points fall outside the voids \cite{34}. Table 1 presents the max, min, and average of the N-point probability function for 100 randomly generated microstructures. The total number of trials to extract the N-point probability functions (1-point, 2-point, 3-point, respectively) is 1000, which is accepted as enough based on our preliminary study.

![Figure 3.](a) 1-point probability function: the red points are inside the voids, and the blue points are outside of voids, the fraction of red points (void space) to the sum of red and blue points (total volume) called 1-point probability function, (b) 2-point probability function: two points are randomly tossed, and the event when all 2 points fall outside voids is considered, (c) 3-point probability function: three points are randomly tossed in microstructures, and the event when 3 points fall outside voids is considered, (d) lineal-path probability function: the probability when the whole line is positioned inside voids.

Table 1. Minimum, maximum, and average of 4 probabilistic descriptors for 100 microstructures.

| Statistical Ensemble | 1 PF       | 2 PF       | 3 PF       | LPF        |
|----------------------|------------|------------|------------|------------|
| Average              | 0.38758    | 0.38895    | 0.24738    | 0.14744    |
| Max                  | 0.598      | 0.604      | 0.453      | 0.331      |
| Min                  | 0.229      | 0.175      | 0.071      | 0.054      |

3.2.2. Lineal-Path Function

In the preceding section, the N-point probability functions are implemented to characterize the geometrical heterogeneity of microstructures concerning the porosity and distribution of voids. A lineal-path function is further implemented as an additional descriptor to account for the level of convexity of voids. The lineal-path function \cite{35} is also defined as a probability of a randomly generated line associated with the voids (Figure 3). Specifically, a line can be drawn by connecting two points, that are randomly generated as the 2-point probability function. This lineal-path naturally has a randomly generated length and alignment. The probability then can be determined when the whole line locates inside of any voids. Likewise, 1000 randomly populated linear lines are used for each microstructure.
Table 1 summarizes the max, min and average values of four geometrical descriptors for 100 randomly generated microstructures.

3.3. Generation of Loading Path

On top of different microstructures for geometrical heterogeneity, the selection of loading paths is crucial for obtaining diverse microstructural responses. In other words, the homogenized behaviors from micro-level simulations under selected loading paths should include all potential mechanical responses that a data-driven model should learn. Since the supervised learning is utilized, a pattern between input and target data is extracted based on the available pattern of the database. Therefore, the database should include all the patterns of microstructural responses.

There are multiple loading conditions, for instance, monotonic, biaxial, cyclic, etc. Furthermore, each loading method yields specific responses of microstructures. Either using lab testing or machine learning, however, technically, it is impossible to consider all potential loading behaviors. Therefore, we may identify the possible scenarios of loading conditions to analyze the material’s behavior properly.

In this study, we adopt a random generation method, which is one of the most common approaches to populate data. As input for describing microstructural behavior, the randomly generated strain values are used. Under the given strain value, which is converted to the displacement boundary condition to the microscopic domain, the micro-level FEM simulation yields the homogenized stress (Please refer to Section 2.1). In other words, the sequence of loading paths is obtained, which consists of a pair of stress–strain values after running micro-level fem simulations.

Sampling a temporal loading path is challenging since a random path (rather than a single point) should be generated. If the random strain values are considered for every loading step in a loading path, a smooth loading path may not be guaranteed because of the nature of the random generation method. In other words, a loading path with fully generated by random strain values will be highly oscillating and lacking the natural trend of loading paths under the static condition. To deal with this potential issue, instead of generating random strains for all loading steps, randomly generated strains are only assigned to 6 equally spaced loading steps (our selected steps are 0, 20, 40, 60, 80, 100). Then, the 94 strains are considered for loading via a fitted six-degree polynomial to those above 6 random points [24], where an example of a loading path is depicted in Figure 4.

Figure 4. Six random numbers are generated for the loading step at 0, 20, 40, 60, 80, and 100. A six-degree polynomial fitted to these random numbers to smooth the generated path-using polynomial 100 data are generated (X-axis is time step and Y-axis is strain).
The design of the experiment (DOE) depends on the complexity of the target behavior. Table 2 depicts details of DOE for linear and nonlinear elastic problems.

Table 2. Design of experiment for learning response of heterogeneous microstructure.

| Parameters | Linear | Nonlinear |
|------------|--------|-----------|
| Heterogeneity | Geometric and Material Properties | Geometric |
| Number of Microstructure | 100 | 20 |
| Number of Loading Path | 20 | 20 |
| Number of Loading Steps | 100 | 20 |
| Strain Value | −0.05–0.05 | −0.005–0.005 |

4. Numerical Problems

In this section, the capability of a data-driven computational homogenization method is presented for linear and nonlinear (hypoelastic) heterogeneous microstructures. For each case, the design of experiment (DOE) is referred to Section 3. It is worth noting that the number of microstructures and training paths are different for linear and nonlinear conditions because of each problem’s difference in the level of complexity (see Table 2).

4.1. Training and Validation of Linear-Elastic Responses for Heterogeneous Microstructures

The behavior of elastic porous microstructures highly depends on the geometry and material properties of microstructures. Figure 5a,b, which are obtained from homogenization via FE², depict geometrical and material heterogeneity dependent behaviors, respectively. This study aims to learn homogenized responses of heterogeneous microstructures originated from both material properties and geometrical features.

![Figure 5](image-url)

(a) Stress (GPa) vs. strain (b) Stress (GPa) vs. strain

Figure 5. (a) Comparison of homogenized behavior (Linear) of 3 microstructures under monotonic loading, the geometrical features for these 3 microstructures are [0.358, 0.455, 0.278, 0.178], [0.313, 0.465, 0.36, 0.226], [0.478, 0.28, 0.143, 0.064] (1-point, 2-point, 3-point, and Linear-path probabilistic functions, respectively), (b) comparison of homogenized behaviour (Linear) of 1 microstructure with different material properties ([0.358, 0.455, 0.278, 0.178] are 1-point, 2-point, 3-point, and linear-path probabilistic functions, respectively) under monotonic loading.

As in Table 2, the homogenized responses of randomly generated 100 microstructures are obtained under 20 loading paths (20 loading steps for each loading path) with the strain range of (−0.05–0.05). In order to consider the heterogeneity of material properties, this procedure is repeated by setting the first lame coefficient equal to \(\lambda = 200 \text{ GPa}\) and the second lame coefficient (\(\mu\)) equal to 20, 30, 50, or 70 GPa. Figure 6 depicts a diagram of loading procedure and the generation of data.
Figure 6. Data generation for linear problem. Twenty loading paths are applied to every microstructure, then the material properties are changed, and the process is repeated.

As described in the preceding section, four descriptors (1-point, 2-point, 3-point, and linear-path) are introduced to characterize the geometrical features of microstructures. The material properties and three components of strains are further added as input to establish our neural networks, which are based on simple Artificial Neural Networks (ANN). The training procedure is leveraged by Keras [36] with a TensorFlow [37] backend. Table 3 demonstrates the architecture of the ANN for which ADAM optimizer and mean absolute error (MAE) are considered for training with 200 epochs.

Table 3. The architecture of network for learning linear problem.

| Layer (Type) | Output Shape | Activation Function |
|--------------|--------------|---------------------|
| Input        | (None, 6)    | None                |
| Dense        | (None, 100)  | Relu                |
| Dense        | (None, 80)   | Relu                |
| Dense        | (None, 60)   | Relu                |
| Dense        | (None, 40)   | Relu                |
| Dense        | (None, 20)   | Relu                |
| Dense        | (None, 10)   | Relu                |
| Output       | (None, 3)    | tanh                |

For testing of a trained model, new three random microstructures (Figures 7a, 8a and 9a) and new three random loading paths (Figures 7d, 8d and 9d) are generated, which are not previously used for training. At the test 1 and test 2, Figures 7 and 8, the material properties are $\lambda = 200$ GPa, and $\mu = 25$ GPa. For the third problem, Figure 9, the second lame coefficient is equal to $\mu = 55$ GPa and $\lambda = 200$ GPa; therefore, the heterogeneity in terms of both microstructural geometry and material properties is considered. Figures 7e, 8e and 9e present a comparison between the homogenized response of microstructures via FE$^2$ framework and trained model under newly generated strain path (Figures 7d, 8d and 9d, respectively). The results demonstrate that all three stress responses $\sigma_{xx}$ (green), $\sigma_{yy}$ (blue) and $\sigma_{xy}$ (red) are captured with only 2 percent errors. Note that mean squared error is considered.
Figure 7. Test 1 for homogenization of linear elastic microstructure ($\mu = 25$ GPa and $\lambda = 200$ GPa), (a) FEM mesh, (b) X displacement (initial step), (c) Y displacement (initial step), (d) random generated strain, and (e) comparison of homogenized effective stress and Data-Driven responses.

Figure 8. Test 2 for homogenization of linear elastic microstructure ($\mu = 25$ GPa and $\lambda = 200$ GPa), (a) FEM mesh, (b) X displacement (initial step), (c) Y displacement (initial step), (d) random generated strain, and (e) comparison of homogenized effective stress and data-driven responses.
4.2. Training and Validation of Hypoelastic Responses for Heterogeneous Microstructures

In this problem, the nonlinear (hypoelastic) elastic responses of microstructures are further considered associated with geometrical heterogeneity. Firstly, Figure 10 depicts the nonlinear behavior of three different microstructures (with the same material properties). As presented in Table 2, it is worth noting that only the geometrical heterogeneity is considered. The mechanical responses of 20 microstructures under 20 loading paths within the strain range of (−0.005 to +0.005) are collected for the database.

![Figure 10. Comparison of homogenized behavior of 3 microstructures under monotonic loading, the geometrical features for these 3 microstructures are [0.358, 0.455, 0.278, 0.178], [0.313, 0.465, 0.36, 0.226], [0.478, 0.28, 0.143, 0.064] (respectively, first, second, third and linear path probabilistic functions). By changing the microstructure, there are different behaviors (Stress (GPa) vs. Strain).](image-url)
In this problem, it is worth noting that the past three strains are considered, where their average is adopted as input to account for nonlinearity. Likewise, the linear elasticity, three components of the current strain, and four geometrical descriptors are fed into the ANN. The architecture of the network is demonstrated in Table 4, for which ADAM optimizer and mean absolute error are considered for 500 epochs training.

Table 4. The architecture of network for learning nonlinear problem.

| Layer (Type) | Output Shape | Activation Function |
|--------------|--------------|---------------------|
| Input        | (None, 6)    | None                |
| Dense        | (None, 100)  | Relu                |
| Dense        | (None, 80)   | Relu                |
| Dense        | (None, 60)   | Relu                |
| Output       | (None, 3)    | tanh                |

To test the trained model, the behavior of the trained model examined by three new random porous microstructures (Figures 11a, 12a and 13a) under a new random loading path (Figures 11d, 12d and 13d). At the first and second problems, a random new microstructure is generated, and a new random loading path is applied onto it (Figures 11 and 12). The third problem of this section considered the prediction of monotonic loading (Figure 13). Figures 11e, 12e and 13e depict a comparison between homogenized response of microstructure via FE and trained model. The results demonstrate all three stress responses $\sigma_{xx}$ (green), $\sigma_{yy}$ (blue) and $\sigma_{xy}$ (red) are captured with only 2 percent errors, it is worth noting that the error is calculated via mean squared function.

Figure 11. Test 1 for homogenization of nonlinear microstructure ($\mu = 55$ GPa and $\lambda = 200$ GPa), (a) FEM mesh, (b) X displacement (initial step), (c) Y displacement (initial step), (d) random generated strain, and (e) comparison of homogenized effective stress and data-driven responses.
Figure 12. Test 2 for homogenization of nonlinear microstructure ($\mu = 55$ GPa and $\lambda = 200$ GPa), (a) FEM mesh, (b) X displacement (initial step), (c) Y displacement (initial step), (d) random generated strain, and (e) comparison of the homogenized effective stress and the data-driven responses.

Figure 13. Test 3 for homogenization of nonlinear microstructure ($\mu = 55$ GPa and $\lambda = 200$ GPa), (a) FEM mesh, (b) X displacement (initial step), (c) Y displacement (initial step), (d) random generated strain, and (e) comparison of the homogenized effective stress and the data-driven responses.
Since the process of learning was not challenging, and considering microstructure descriptors, the unique mapping between input and output can be constructed, the hyper-parameters are optimized using a simple trial and error method by minimizing the model error, which can be used when the problem is not complex and easy to handle (babysitting hyper-parameter tuning).

5. Discussion

The results in the previous section presents the ability of machine learning (deep-neural network) to predict the homogenized mechanical responses of heterogeneous microstructures when constitutive laws of materials are assumed (1) linear elastic (Problem 1) and (2) nonlinear hypoelastic (Problem 2). The database for training are constructed based on the homogenization of heterogeneous porous microstructure using FE framework, and the level of heterogeneity for each problem is presented in Table 2.

A deep neural network is designed to predict the microstructural behavior by feeding the loading path and geometrical descriptors of each microstructure (Table 1). One of the challenges in predicting mechanical responses via deep learning is the process of learning behavior then over-fitting the database used for training. Therefore, to demonstrate the fact that the trained deep neural network captures the linear and nonlinear behavior, we test the model with both random and monotonic (Figure 13) loading paths. The loading path is generated in Section 3.3 and consists of three strain components, which are presented with a different colors. The responses of the deep network and elastic models are compared, and there is a negligible difference. Such a homogenization scheme is highly valuable to speed up the simulation time of multiscale frameworks without loss of information during modeling of heterogeneous system.

6. Conclusions

Spatially varying porosity highly affects the mechanical behavior of porous materials like soil and cast aluminum alloys. Multiscale modeling approaches have been developed to consider such heterogeneity associated with different material properties. However, these methods require expensive computational costs in general. This study develops a computational homogenization scheme for heterogeneous elastic porous solids based on Artificial Intelligence. This intelligent homogenization framework aims to replace demanding micro-level FE simulations by leveraging a data-driven model that is trained via an off-line method. The overall innovation of this study is implementing deep learning to predict the mechanical behavior of heterogeneous elastic microstructures. Our starting point is to construct a database for training through a number of micro-level FE experiments, which yield homogenized microstructural responses—a pair of strain and stress values. A random generation method is adopted to include potential heterogeneous responses associated with the loading path, microstructures, and material properties. In particular, four probability-based descriptors representing the geometrical heterogeneity of microstructures are introduced as input features for machine learning. Both linear and nonlinear elastic responses are tested to demonstrate the performance of the proposed computational homogenization approach. Our results indicate that a simple neural network can capture various elastic responses of heterogeneous microstructures when proper input features are selected on top of the integrated database based on the random generation method.

Author Contributions: Conceptualization, method, writing—original, E.M.H.; Conceptualization, writing—original draft, review, editing, supervision, S.N. Both authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Natural Sciences and Engineering Research Council of Canada (NSERC).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.
Data Availability Statement: The data presented in this study are available on request from the corresponding author.

Acknowledgments: This research is supported by Natural Sciences and Engineering Research Council of Canada (NSERC). These supports are gratefully acknowledged.

Conflicts of Interest: The authors declare no conflict of interest.

Nomenclature
The following variables are used in this manuscript:

\( \sigma_M \) Macro Stress
\( \nabla \) Differential Operator
\( \Omega_M \) Macro-Level Space
\( \Gamma_M^u \) Dirichlet Boundary
\( \Gamma_M^N \) Neumann Boundary
\( \varepsilon_M \) Macro Strain
\( \mathbb{N}(\cdot) \) Micro-Level Simulation
\( N_M^T \) Macro-Level Shape Function
\( B_M \) Derivative of Macro-Level Shape Function
\( D_M \) Macro Consistent Tangent
\( \varepsilon_M \) Macroscopic Strain
\( x_q \) Boundary Node Displacement Matrix of the RVE
\( \mathbb{D}_q \) Matrix Depends on the Coordinate of Nodal Points in the RVE of Microstructures
\( x \) Displacement at the Micro-Level
\( \sigma_m \) Stress at the Micro-Level
\( \Omega_m \) Volume of the RVE of Microstructures
\( \mu \) First Lame’s Coefficient
\( \lambda \) Second Lame’s Coefficient
\( E \) Young’s Modulus
\( \nu \) Poisson’s Ratio
\( x_a \) Exterior Nodes
\( \mathcal{V} \) RVE Associated with Microstructures
\( C \) Homogenized Tangent Stiffness
\( \mathcal{V} \) Volume of the RVE of Microstructures
\( \eta \) Learning Rate
\( \delta_j \) Gradient of the Total Error with Respect to Net Input at Unit j
\( \Phi' \) Derivative of the Activation Function
\( \mathcal{L}^{(i)}(x) \) Indicator Function
\( \mathbb{F} \) Expectation Value of any Function
FEM Finite Element Method
\( \text{FE}^2 \) Double Scale Finite Element Method
RVE Representative Volume Element
POD Proper Orthogonal Decomposition
TFA Transformation Filed Analysis
FFTH Fast Fourier Transform Homogenization
AI Artificial Intelligence
ANN Artificial Neural Network
LSTM Long-Short Term Memory Unit
DOE Design of Experiment
DL Deep Learning
ADAM Optimizer
MAE Mean Absolute Error

References
1. Feyel, F.; Chaboche, J.L. \text{FE}^2 multiscale approach for modelling the elastoviscoplastic behaviour of long fibre SiC/Ti composite materials. \textit{Comput. Methods Appl. Mech. Eng.} \textbf{2000}, \textit{183}, 309–330. [CrossRef]
2. Liu, Y.; Sun, W.; Yuan, Z.; Fish, J. A nonlocal multiscale discrete-continuum model for predicting mechanical behavior of granular materials. \textit{Int. J. Numer. Methods Eng.} \textbf{2016}, \textit{106}, 129–160. [CrossRef]
3. Wang, K.; Sun, W. A semi-implicit discrete-continuum coupling method for porous media based on the effective stress principle at finite strain. *Comput. Methods Appl. Mech. Eng.* **2016**, *304*, 546–583. [CrossRef]

4. Na, S.; Sun, W. Computational thermomechanics of crystalline rock, Part I: A combined multi-phase-field/crystal plasticity approach for single crystal simulations. *Comput. Methods Appl. Mech. Eng.* **2018**, *338*, 657–691. [CrossRef]

5. Geers, M.; Yvonnet, J. Multiscale thermomechanics of crystalline rock, Part I: A combined multi-phase-field/crystal plasticity approach for single crystal simulations. *Comput. Methods Appl. Mech. Eng.* **2018**, *338*, 657–691. [CrossRef]

6. Foygel, F. Multiscale FE2 elastoviscoplastic analysis of composite structures. *Comput. Mater. Sci.* **1999**, *16*, 344–354. [CrossRef]

7. Kanit, T.; Forest, S.; Galliet, I.; Mouly, Y.; Jeulin, D. Determination of the size of the representative volume element for random composites: Statistical and numerical approach. *Int. J. Solids Struct.* **2003**, *40*, 3647–3679. [CrossRef]

8. Di, Z.; Luo, Z.; Xie, Z.; Wang, A.; Navon, I. An optimizing implicit difference scheme based on proper orthogonal decomposition for the two-dimensional unsaturated soil water flow equation. *Int. J. Numer. Methods Fluids* **2012**, *68*, 1324–1340. [CrossRef]

9. Jolliffe, I.T.; Cadima, J. Principal component analysis: A review and recent developments. *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.* **2016**, *374*, 20150202. [CrossRef]

10. Rajaee, M.; Karlsson, S.K.; Sirovich, L. Low-dimensional description of free-shear-flow coherent structures and their dynamical behaviour. *J. Fluid Mech.* **1994**, *258*, 1–29. [CrossRef]

11. Dvorak, G.; Rao, M.M. Axisymmetric plasticity theory of fibrous composites. *Int. J. Eng. Sci.* **1976**, *14*, 361–373. [CrossRef]

12. Dvorak, G.; Bahet-El-Din, Y.; Wafa, A. The modeling of inelastic composite materials with the transformation field analysis. *Model. Simul. Mater. Sci. Eng.* **1994**, *2*, 571. [CrossRef]

13. Mounine, H.; Suquet, P. A fast numerical method for computing the linear and nonlinear mechanical properties of composites. In *Comptes Rendus de l’Académie des Sciences*; Série II. Mécanique, physique, chimie, astronomie; HAL: Lyon, France, 1994. Available online: https://hal.archives-ouvertes.fr/hal-00000000/document (accessed on 23 July 2021).

14. Staszak, N.; Garbowski, T.; Szyczak-Graczyk, A. Solid-Truss to Shell Numerical Homogenization of Prefabricated Composite Slabs. 2021. Available online: https://www.mdpi.com/1996-1944/14/15/4120/htm (accessed on 23 July 2021).

15. Garbowski, T.; Knitter-Platkowska, A.; Mrówczyński, D. Numerical Homogenization of Multi-Layered Corrugated Cardboard with Creasing or Perforation. 2021. Available online: https://www.mdpi.com/1996-1944/14/3786 (accessed on 6 July 2021).

16. McCarthy, J. What Is Artificial Intelligence? 1998. Available online: http://cogprints.org/412/2/whatisai.ps (accessed on 6 July 2021).

17. Turing, A.M.; Hauqeland, J. *Computing Machinery and Intelligence*; MIT Press: Cambridge, MA, USA, 1950.

18. Ghaboussi, J.; Garrett, J., Jr.; Wu, X. Knowledge-based modeling of material behavior with neural networks. *J. Eng. Mech.* **1991**, *117*, 132–153. [CrossRef]

19. Ghaboussi, J.; Pecknold, D.A.; Zhang, M.; Haj-Ali, R.M. Autoprogressive training of neural network constitutive models. *Int. J. Numer. Methods Eng.* **1998**, *42*, 105–126. [CrossRef]

20. Zhu, J.H.; Zaman, M.M.; Anderson, S.A. Modeling of soil behavior with a recurrent neural network. *Can. Geotech. J.* **1998**, *35*, 858–872. [CrossRef]

21. Huber, N.; Tsakmakis, C. Determination of constitutive properties from spherical indentation data using neural networks. Part I: The case of pure kinematic hardening in plasticity laws. *J. Mech. Phys. Solids* **1999**, *47*, 1569–1588. [CrossRef]

22. Pernot, S.; Lamarque, C.H. Application of neural networks to the modelling of some constitutive laws. *Neural Netw.* **1999**, *12*, 371–392. [CrossRef]

23. Haj-Ali, R.; Pecknold, D.A.; Ghaboussi, J.; Voiyadjis, G.Z. Simulated micromechanical models using artificial neural networks. *J. Eng. Mech.* **2001**, *127*, 730–738. [CrossRef]

24. Mozaffar, M.; Bostanabad, R.; Chen, W.; Ehmann, K.; Cao, J.; Bessa, M. Deep learning predicts path-dependent plasticity. *Proc. Natl. Acad. Sci. USA* **2019**, *116*, 26414–26420. [CrossRef]

25. Ali, U.; Muhammad, W.; Brahme, A.; Skiba, O.; Inal, K. Application of artificial neural networks in micromechanics for polycrystalline metals. *Int. J. Plast.* **2019**, *120*, 205–219. [CrossRef]

26. Wang, K.; Sun, W.; Du, Q. A cooperative game for automated learning of elasto-plasticity knowledge graphs and models with AI-guided experimentation. *Comput. Mech.* **2019**, *64*, 467–499. [CrossRef]

27. Ghavamian, F.; Simone, A. Accelerating multiscale finite element simulations of history-dependent materials using a recurrent neural network. *Comput. Methods Appl. Mech. Eng.* **2019**, *357*, 112594. [CrossRef]

28. Capuano, G.; Rimoli, J.J. Smart finite elements: A novel machine learning application. *Comput. Methods Appl. Mech. Eng.* **2019**, *345*, 363–381. [CrossRef]

29. Miehe, C.; Koch, A. Computational micro-to-macro transitions of discretized microstructures undergoing small strains. *Arch. Appl. Mech.* **2002**, *72*, 300–317. [CrossRef]

30. Kouznetsova, V.; Geers, M.G.; Brekelmans, W.M. Multi-scale constitutive modelling of heterogeneous materials with a gradient-enhanced computational homogenization scheme. *Int. J. Numer. Methods Eng.* **2002**, *54*, 1235–1260. [CrossRef]

31. Bower, A.F. *Applied Mechanics of Solids*; CRC Press: Boca Raton, FL, USA, 2009.

32. Cunningham, P.; Cord, M.; Delany, S.J. Supervised learning. In *Machine Learning Techniques for Multimedia*; Springer: Berlin, Germany, 2008; pp. 21–49.

33. Nair, V.; Hinton, G.E. Rectified linear units improve restricted boltzmann machines. In Proceedings of the ICML, Haifa, Israel, 21–24 June 2010.
34. Torquato, S.; Haslach, H., Jr. Random heterogeneous materials: Microstructure and macroscopic properties. *Appl. Mech. Rev.* **2002**, *55*, B62–B63. [CrossRef]

35. Lu, B.; Torquato, S. Lineal-path function for random heterogeneous materials. *Phys. Rev. A* **1992**, *45*, 922. [CrossRef] [PubMed]

36. Chollet, F. Keras. 2015. Available online: https://keras.io (accessed on 6 July 2021).

37. Abadi, M.; Agarwal, A.; Barham, P.; Brevdo, E.; Chen, Z.; Citro, C.; Corrado, G.S.; Davis, A.; Dean, J.; Devin, M.; et al. TensorFlow: Large-Scale Machine Learning on Heterogeneous Systems. 2015. Available online: https://www.tensorflow.org (accessed on 6 July 2021).